

## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	3	(("2882323") or ("5872277") or ("6278016")).PN.	US-PGPUB; USPAT	OR	OFF	2007/05/30 12:48
L2	1	DE-3021414-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:49
L3	2	DE-3105399-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:51
L4	1	GB-1341015-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:51
L5	2	GB-2051067-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:52
L6	2	JP-60239443-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:52
L7	0	WO-2000026175-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:53
L8	1	WO-200026175-\$ did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:54
L9	1105	diene near3 carboxylic adj acid	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:54
L10	454	I9 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:55
L11	363	myrcene near5 isoprene	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:56
L12	257	I11 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:56

## EAST Search History

L13	399	myrcene near5 isoprene	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:56
L14	257	l13 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:07
L15	0	l10 and  l14	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:03
L16	18353	"alkanoic acids"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:06
L17	605	"alkanoic acids".ti.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:08
L18	268	l17 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:08
L19	0	l14 and  l18	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:07
L20	2636	"alkanoic acids".ti.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:08
L21	268	l20 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:09
L22	1	l21 and myrcene	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:09
L23	109	ester near5 diene adj compound	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:09
L24	67	l23 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:10
S1	239	"560/249".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 10:30

## EAST Search History

S2	21	((JAMES) near2 (BABLER)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/29 14:58
S3	3	((JAMES) near2 (BABLER)).INV.	EPO; JPO; DERWENT	OR	ON	2007/05/29 14:58
S4	239	"560/249".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/29 15:01
S5	61	S4 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:55
S6	1	("5872277").PN.	US-PGPUB; USPAT	OR	OFF	2007/05/30 10:30
S7	1	("5872277").URPN.	USPAT	OR	ON	2007/05/30 11:44
S8	0	GB-1172516-\$ did.	USPAT	OR	ON	2007/05/30 11:45
S9	0	GB-1172516-\$ did.	US-PGPUB; USPAT; USOCR; EPO	OR	ON	2007/05/30 12:47

SEARCH HISTORY

=&gt; d his nofile

mwi  
5/26/07

(FILE 'HOME' ENTERED AT 10:23:49 ON 16 MAY 2007)

FILE 'HCAPLUS' ENTERED AT 10:24:09 ON 16 MAY 2007  
E US20070055076/PNL1 1 SEA ABB=ON PLU=ON US20070055076/PN  
D ALL  
SEL RNFILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007  
L2 35 SEA ABB=ON PLU=ON (100-66-3/BI OR 105-87-3/BI OR  
105-90-8/BI OR 105-91-9/BI OR 106-24-1/BI OR 106-25-2/B  
I OR 106-42-3/BI OR 107-92-6/BI OR 108-21-4/BI OR  
108-88-3/BI OR 108-90-7/BI OR 108-94-1/BI OR 109-20-6/B  
I OR 1191-16-8/BI OR 123-35-3/BI OR 123-86-4/BI OR  
127-08-2/BI OR 127-09-3/BI OR 137-40-6/BI OR 138-86-3/B  
I OR 141-12-8/BI OR 142-96-1/BI OR 157258-67-8/BI OR  
19559-59-2/BI OR 3915-83-1/BI OR 503-74-2/BI OR  
5392-40-5/BI OR 556-82-1/BI OR 64-19-7/BI OR 78-79-5/BI  
OR 78-93-3/BI OR 79-09-4/BI OR 79-31-2/BI OR 80-26-2/B  
I OR 851785-97-2/BI)L3 19 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS  
D SCANL4 1 SEA ABB=ON PLU=ON 123-35-3/RN  
D SCAN  
D IDEL5 1 SEA ABB=ON PLU=ON 78-79-5/RN  
D SCAN  
D IDEL6 1 SEA ABB=ON PLU=ON 1191-16-8/RN  
D SCAN  
D CN  
D IDEL7 1 SEA ABB=ON PLU=ON 105-87-3/RN  
D SCAN  
D IDEL8 1 SEA ABB=ON PLU=ON 141-12-8/RN  
D IDE

L9 11 SEA ABB=ON PLU=ON L2 AND ?ACETATE?/CNS

FILE 'STNGUIDE' ENTERED AT 10:44:21 ON 16 MAY 2007

FILE 'CASREACT' ENTERED AT 10:50:09 ON 16 MAY 2007

L10 1 SEA ABB=ON PLU=ON 123-35-3/RCT(L) (105-87-3/PRO OR  
141-12-8/PRO)  
D SCANL11 2 SEA ABB=ON PLU=ON 78-79-5/RCT(L) 1191-16-8/PRO  
D SCAN  
E ESTER/CT  
E ESTERS/CTL12 23 SEA ABB=ON PLU=ON 64-19-7/RCT(L) (123-35-3/RCT OR  
78-79-5/RCT)  
D SCAN

L13 STR 123-35-3

L14 36 SEA SSS SAM L13 ( 448 REACTIONS)

L15 789 SEA SSS FUL L13 ( 11229 REACTIONS)

SAV L15 LAO307CRCT/A

E ESTERS/CT

L16 7147 SEA ABB=ON PLU=ON ESTERS+PFT, OLD, NT/CT

L17 7 SEA ABB=ON PLU=ON L15 AND L16

D SCAN

D SCAN

D QUE

SAV L17 LAO307CRCTA/A  
 L18 STR L13  
 L19 6 SEA SUB=L15 SSS SAM L18 ( 28 REACTIONS)  
 D SCAN  
 L20 88 SEA SUB=L15 SSS FUL L18 ( 708 REACTIONS)  
 SAV L20 LAO307CRCTB/A  
 L21 STR L18  
 L22 1 SEA SUB=L15 SSS SAM L21 ( 7 REACTIONS)  
 D SCAN  
 L23 5 SEA SUB=L15 SSS FUL L21 ( 16 REACTIONS)  
 D SCAN  
 SAV L23 LAO307CRCTC/A  
 L24 STR L21  
 L25 1 SEA SUB=L15 SSS SAM L24 ( 7 REACTIONS)  
 D SCAN  
 L26 7 SEA SUB=L15 SSS FUL L24 ( 38 REACTIONS)  
 D SCAN  
 SAV L26 LAO307CRCTD/A  
 SAV L27 LAO307CRCTE/A  
 L27 34 SEA ABB=ON PLU=ON (L10 OR L11 OR L12) OR L17 OR L23  
 OR L26  
 L28 43 SEA ABB=ON PLU=ON BABLER JAMES?/AU  
 L29 3 SEA ABB=ON PLU=ON L27 AND L28  
 SAV L29 LAO307CRCTIN/A  
 L30 31 SEA ABB=ON PLU=ON L27 NOT L29

FILE 'HCAPLUS' ENTERED AT 12:06:06 ON 16 MAY 2007

L31 QUE ABB=ON PLU=ON PY<2004 OR PRY<2004 OR AY<2004 OR  
 MY<2004 OR REVIEW/DT  
 L32 1 SEA ABB=ON PLU=ON L1 AND L31  
 D SCAN

FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007

L33 25 SEA ABB=ON PLU=ON L30 AND L31  
 L34 3 SEA ABB=ON PLU=ON L29 AND L31

FILE 'HCAPLUS' ENTERED AT 12:08:48 ON 16 MAY 2007

D SCAN L1  
 L35 619 SEA ABB=ON PLU=ON L4/RACT  
 L36 5537 SEA ABB=ON PLU=ON L5/RACT  
 L37 86 SEA ABB=ON PLU=ON L6/P  
 L38 347 SEA ABB=ON PLU=ON L7/P  
 D 1-2 KWIC  
 L39 144 SEA ABB=ON PLU=ON L8/P  
 D KWIC  
 D 1-2 L36 KWIC  
 L40 0 SEA ABB=ON PLU=ON L36(L) L37  
 L41 12 SEA ABB=ON PLU=ON L36 AND L37  
 L42 0 SEA ABB=ON PLU=ON L35(L) (L38 OR L39)  
 L43 10 SEA ABB=ON PLU=ON L35 AND (L38 OR L39)  
 L44 20 SEA ABB=ON PLU=ON (L40 OR L41 OR L42 OR L43)  
 L45 34845 SEA ABB=ON PLU=ON L9  
 L46 70 SEA ABB=ON PLU=ON (L35 OR L36) AND L45  
 L47 4036 SEA ABB=ON PLU=ON L9/RACT  
 L48 50 SEA ABB=ON PLU=ON (L35 OR L36) AND L47  
 L49 9 SEA ABB=ON PLU=ON L48 AND L44  
 E ESTERS/CT  
 L50 QUE ABB=ON PLU=ON ESTERS+PFT,OLD,NT1/CT  
 L51 70 SEA ABB=ON PLU=ON L44 OR L46 OR (L48 OR L49)  
 L52 47 SEA ABB=ON PLU=ON L51 AND L50  
 E VITAMINS/CT  
 L53 QUE ABB=ON PLU=ON VITAMINS+PFT,OLD,NT/CT  
 E FLAVOR/CT  
 E FLAVORS/CT  
 E FLAVORING/CT  
 L54 QUE ABB=ON PLU=ON FLAVOR+PFT,OLD,NT/CT

L55           3 SEA ABB=ON PLU=ON L51 AND (L53 OR L54)  
           D SCAN  
           D SCAN L1  
           E "DIETARY SUPPLEMENTS"/CT  
 L56           QUE ABB=ON PLU=ON "DIETARY SUPPLEMENTS"+PFT,OLD,NT/CT  
 L57           QUE ABB=ON PLU=ON "FLAVORING MATERIALS"+PFT,OLD,NT/CT  
 L58           QUE ABB=ON PLU=ON "ODOR AND ODOROUS SUBSTANCES"+PFT,O  
           LD,NT/CT  
 L59           45 SEA ABB=ON PLU=ON L52 AND L31  
           SAV L59 LAO307HCP/A  
 L60           43 SEA ABB=ON PLU=ON L28  
           D QUE  
 L61           43 SEA ABB=ON PLU=ON L60 AND L31  
 L62           QUE ABB=ON PLU=ON VITAM? OR ODOR? OR SMELL? OR  
           PERFUM? OR SUPPLEMENT? OR FLAVOR?  
 L63           4 SEA ABB=ON PLU=ON L61 AND L62  
 L64           4 SEA ABB=ON PLU=ON L61 AND (L53 OR L56 OR L57 OR L58)  
           D QUE  
 L65           5 SEA ABB=ON PLU=ON L51 AND (L53 OR L56 OR L57 OR L58)  
 L66           45 SEA ABB=ON PLU=ON L55 OR L59 OR L65  
 L67           45 SEA ABB=ON PLU=ON L66 AND L31  
           SAV L67 LAO307HCP/A  
 L68           6 SEA ABB=ON PLU=ON L63 OR L64  
 L69           13 SEA ABB=ON PLU=ON L61 AND L50  
 L70           17 SEA ABB=ON PLU=ON L68 OR L69  
           SAV L70 LAO307HCPIN/A  
           D QUE L67  
 L71           43 SEA ABB=ON PLU=ON L67 NOT L70  
           D QUE L34  
           D QUE L33

FILE 'CASREACT' ENTERED AT 12:45:36 ON 16 MAY 2007  
       D QUE L33

FILE 'STNGUIDE' ENTERED AT 12:46:03 ON 16 MAY 2007

FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16  
   MAY 2007

L72           4 SEA ABB=ON PLU=ON L28  
           D 1-4 TI  
           SAV L72 LAO307IN/A

FILE 'STNGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007  
       D QUE L34  
       D QUE L70  
       D QUE L72

FILE 'CASREACT, HCAPLUS, BIOSIS' ENTERED AT 12:49:46 ON 16 MAY  
   2007

L73           19 DUP REM L34 L70 L72 (5 DUPLICATES REMOVED)  
           ANSWERS '1-3' FROM FILE CASREACT  
           ANSWERS '4-18' FROM FILE HCAPLUS  
           ANSWER '19' FROM FILE BIOSIS

FILE 'CASREACT' ENTERED AT 12:51:20 ON 16 MAY 2007

FILE 'CASREACT, HCAPLUS, BIOSIS' ENTERED AT 12:57:01 ON 16 MAY  
   2007  
       D L73 1-19 IBIB ABS

FILE 'CASREACT' ENTERED AT 12:57:02 ON 16 MAY 2007

SN 10/S64307 Page 139 of 139 STIC SIN SEARCH 5/17/2007

FILE 'REGISTRY' ENTERED AT 12:57:42 ON 16 MAY 2007

D L4 IDE  
D L5 IDE  
D L6 IDE  
D L7 IDE  
D L8 IDE

FILE 'STNGUIDE' ENTERED AT 12:59:34 ON 16 MAY 2007

D QUE STAT L33  
D QUE STAT L71

FILE 'CASREACT, HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007

L74 67 DUP REM L33 L71 (1 DUPLICATE REMOVED)  
ANSWERS '1-25' FROM FILE CASREACT  
ANSWERS '26-67' FROM FILE HCAPLUS  
D L74 1-25 IBIB ABS FHIT  
D L74 26-67 IBIB ED ABS HITSTR HITIND

**INVENTOR SEARCH**

&gt; d his 134

L23 (FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007)

L24 5 SEA FILE=CASREACT SUB=L15 SSS FUL L21 ( 16 REACTIONS

)

STR

L14 (FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007)  
 => d que 134  
 1 SEA FILE=CASREACT ABB=ON PLU=ON 123-35-3/RCT(L) (105-8  
 7-3/PRO OR 141-28/PRO)  
 L11 2 SEA FILE=CASREACT ABB=ON PLU=ON 78-79-5/RCT(L) (1191-16  
 -8/PRO  
 L12 23 SEA FILE=CASREACT ABB=ON PLU=ON 64-19-7/RCT(L) (123-35  
 -3/RCT OR 78-79-5/RCT)

L13 STR  
 RCT 10  
  
 G1 16 RCT  
 $\text{N}_7\text{C}_2\text{H}$   
 N7-C2H

VAR G1=5/12

NODE ATTRIBUTES:  
CONNECT IS E1 RC AT 17DEFAULT MLEVEL IS ATOM  
MLEVEL IS CLASS AT 2 4 5 6 9 10 11 13 14 15DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1-X7 C AT 17GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18STEREO ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 18STEREO ATTRIBUTES: NONE  
 L25 7 SEA FILE=CASREACT SUB=L15 SSS FUL L24 ( 38 REACTIONS  
 )  
 L27 34 SEA FILE=CASREACT ABB=ON PLU=ON (L10 OR L11 OR L12)  
 OR L17 OR L23 OR L26  
 L28 43 SEA FILE=CASREACT ABB=ON PLU=ON BABLER JAMES?/AU  
 L29 3 SEA FILE=CASREACT ABB=ON PLU=ON L17 AND L28  
 L31 QUE ABB=ON PLU=ON PY<2004 OR PRY<2004 OR AV<2004 OR  
 MY<2004 OR REVIEW/DT  
 L34 3 SEA FILE=CASREACT ABB=ON PLU=ON 129 AND 131

&gt; d his 170

(FILE 'HCAPLUS' ENTERED AT 12:08:48 ON 16 MAY 2007)  
 L17 17 S L68 OR L69  
 L21  
 RCT 10  
  
 G1 16 RCT  
 $\text{N}_7\text{C}_2\text{H}$   
 N7-C2H

L17 (FILE 'HCAPLUS' ENTERED AT 12:08:48 ON 16 MAY 2007)  
 L28 => d que 170  
 L31 43 SEA FILE=CASREACT ABB=ON PLU=ON BABLER JAMES?/AU  
 MI<2004 OR REVIEW/DT  
 L50 QUE ABB=ON PLU=ON ESTERS+PFT,OLD,NT1/CT  
 L53 QUE ABB=ON PLU=ON VITAMINS+PFT,OLD,NT/CT  
 L56 QUE ABB=ON PLU=ON "DIETARY SUPPLEMENTS"+PFT,OLD,NT/C  
 L57 T QUE ABB=ON PLU=ON "FLAVORING MATERIALS"+PFT,OLD,NT/C  
 L58 T QUE ABB=ON PLU=ON "ODOR AND ODOROUS SUBSTANCES"+PFT,  
 OLD,NT/CT  
 L60 43 SEA FILE=HCAPLUS ABB=ON PLU=ON L28  
 L61 43 SEA FILE=HCAPLUS ABB=ON PLU=ON L60 AND L31  
 L62 QUE ABB=ON PLU=ON VITAM? OR ODOR? OR SMELL? OR PERTU  
 M? OR SUPPLEMENT? OR FLAVOR?  
 L63 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND L62  
 L64 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND (L53 OR L56  
 OR L57 OR L58)  
 L68 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L63 OR L64  
 L69 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND L50  
 L70 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L68 OR L69

STEREO ATTRIBUTES: NONE  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 2 4 5 6 9 10 11 13 14 15 17  
 DEFAULT ECLEVEL IS LIMITED  
 GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 18  
 STEREO ATTRIBUTES: NONE

INVENTOR SEARCH RESULTS

=> d his 172  
 (FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16  
 MAY 2007) 4 S L28  
 L72 4 S L28  
 SAV L72 DAO307IN/A

FILE 'STNGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007  
 => dup rem 134 170 172  
 FILE 'CASEACT', ENTERED AT 12:49:46 ON 16 MAY 2007  
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)  
 FILE 'HCAPIUS' ENTERED AT 12:9:16 ON 16 MAY 2007  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

L73 ANSWER 1 OF 19 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 1  
 ACCESION NUMBER: 142:463897 CASREACT Full-text  
 TITLE: Processes for synthesizing esters by  
 1,4-addition of alkanic acids to myrcene or  
 isoprene or

isoprene H.

Babler, James H.

Loyola University of Chicago, USA

PCT Int. Appl., 31 pp.

CODEN: PIXRD2

Patent

English

1

PATENT ASSIGNEE(S):  
 INVENTOR(S):  
 SOURCE:  
 DOCUMENT TYPE:  
 LANGUAGE:  
 FAMILY ACC. NUM. COUNT:  
 PATENT INFORMATION:

## PATENT NO. KIND DATE

WO 2005044774 A1 20050119

WO 2004-US22075 20040708

W. NE, AG, AL, AM, AT, AZ, BA, BB, BG, BR, BW, BY, BZ,  
 CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EG,  
 ES, FI, GB, GD, GE, GH, GM, HR, ID, IL, IN, IS, JP,  
 KE, KG, KR, KZ, LC, IK, LR, LS, LT, LU, LV, MA, MD,  
 MG, MK, MN, MW, MX, NA, NI, NO, NZ, OM, PG, PH, PL,  
 PT, RO, RU, SC, SD, SG, SK, SL, SI, SU, TU, TM, TN, TR,  
 TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RU: BW, GH, GH, KE, US, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,

DE, AZ, BY, KZ, MD, RU, TJ, TM, AT, BE, BG, CH,

CY, CZ, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, IU,

MC, NL, PL, PT, SE, SI, SK, TR, BE, BI, CF, CG, CI,

CM, GA, GN, GO, GR, ML, MR, NE, SN, TD, TG

US 2007055076 A1 20070308

US 2006-564307

20061017

US 2003-486791P

20030711

WO 2004-US22075 20040708

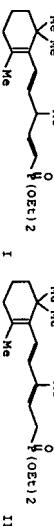
## SN 10/564307 Page 5 of 139 STIC STN SEARCH 5/17/2007

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6278016	A1	20010821	US 1999-458153	19991209
PRIORITY APPLN. INFO.: MARPAT 135:166653 OTHER SOURCE(S): AB				
Methods for preparing ester derivs. of 3-methyl-2-buten-1-ol (prenyl alc.) from the addition reaction of isoprene with alkanoic acids (e.g., acetic acid-acetic anhydride mixture) in the presence of an inorg. acid (e.g., phosphoric acid) catalyst are disclosed. The resultant prenyl ester (e.g., prenyl acetate) readily can be converted to prenyl alc. by saponification				
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT				

L73 ANSWER 3 OF 19 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 84:150125 CASREACT Full-text  
TITLE: A facile route to 2,4-bromo-3-methyl-2-buten-1-ol. Application to the stereoselective synthesis of tri-substituted olefins

AUTHOR(S): Babler, James H.; Buttner, William J.  
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, USA  
SOURCE: Tetrachron Letters (1976), (4), 239-42

DOCUMENT TYPE: Journal  
LANGUAGE: English  
Addition of N-bromosuccinimide to isoprene in AcOH at 25° gave, after fractional distillation, 55%  $\text{AcOCH}_2\text{CH}_2\text{CBr}$  (I, R = H). Reaction of I (R = H, Ac) with BuCuLi gave  $(E)-\text{ROCH}_2\text{CH}_2\text{CMeCH}_2\text{Br}$  (II-Et) and  $\text{BuCH}_2\text{CH}_2\text{CMeCH}_2\text{Br}$ , resp.



L73 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 3  
ACCESSION NUMBER: 2000-123081 HCAPLUS Full-text  
DOCUMENT NUMBER: 132:264887  
TITLE: Method of Preparing 3-(3-methyl-2-buten-1-yl)-2,4-pentandione and Related Dicarbonyl Compounds

INVENTOR(S): Babler, James H.; Posvic, Harvey W.  
SOURCE: Loyola University of Chicago, USA  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:  
PATENT NO. KIND DATE APPLICATION NO. DATE

US 6049010 A 20000411 US 1998-161983 1998-0929

PRIORITY APPLN. INFO.: <--  
OTHER SOURCE(S): CASREACT 132:264987; MARPAT 132:264987  
AB A method for preparation of a dicarbonyl compound by reacting a conjugated alkadiene compound with a 1,3-dicarbonyl compound in the presence of an acid catalyst is

## SN 10/564307 Page 6 of 139 STIC STN SEARCH 5/17/2007

described. E.g., Polyphosphoric acid catalyzed the reaction of 2,4-pentanedione with isoprene to give 59% 3-(3-methyl-2-buten-1-yl)-2,4-pentanedione.

REFERENCE COUNT: 35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L73 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 4  
ACCESSION NUMBER: 1993-124810 HCAPLUS Full-text  
TITLE: An expedient route to a versatile intermediate for the stereoselective synthesis of all-trans-retinoic acid and beta-carotene

AUTHOR(S): Babler, James H.; Schildknecht, Scott A.  
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA  
SOURCE: Tetrahedron Letters (1992), 33(50), 767-700.

DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 118:124810  
GI

CODEN: TELRAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 118:124810  
GI

L73 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1998-021182 HCAPLUS Full-text  
DOCUMENT NUMBER: 122:220459  
TITLE: Methods for preparing prenyl alcohol

INVENTOR(S): Babler, James H.  
SOURCE: Loyola University of Chicago, USA  
CODEN: PCT Int. Appl., 28 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:  
PATENT NO. KIND DATE APPLICATION NO. DATE

WO 9810345 A1 19980917 WO 1998-US256 1998-0108

W: AU, BR, CA, CN, ID, IL, JP, KP, KR, MX, AR, AZ, BY, KG,  
KZ, MD, RU, TJ, TM  
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC,  
NL, PT, SE  
US 5872277 A 19990216 US 1997-814472 1997-0310

CA 2281156 A1 19980917 CA 1998-2281756 &lt;--&gt;

AU 9858171 A 19980929 AU 1998-58171 1998  
0108 <-->EP 988170 A1 20000105 EP 1998-901716 1998  
0108 <-->JP 200114552 T 20010911 JP 1998-539550 1998  
0108 <-->

US 1997-814472 A 1997 0310 &lt;--&gt;

WO 1998-US256 W 1998 0108 &lt;--&gt;

WO 1998-US256 W 1998 0108 &lt;--&gt;

WO 9616013 A1 19980530 WO 1994-339659 1994  
1118 <-->WO 9616013 A1 19980530 WO 1994-339659 1994  
1118 <-->WO 1995-US13372 A1 19980617 WO 1995-US13372 1995  
1011 <-->WO 1995-US13372 A1 19980617 WO 1995-US13372 1995  
1011 <-->

US 1994-339659 A 1994 1118 &lt;--&gt;

WO 1995-US13372 W 1995 1011 &lt;--&gt;

IN THE REFORMAT

REFERENCE COUNT: 4

THERE ARE 4 CITED REFERENCES AVAILABLE

FOR THIS RECORD. ALL CITATIONS AVAILABLE

OTHER SOURCE(S):

L73 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1996-242785 HCAPLUS Full-textDOCUMENT NUMBER: 124:363745 A facile route to 3-alkoxy- $\beta$ -methylpropenals, useful intermediates in the synthesis of carotenoids

AUTHOR(S): Babler, James H.; Liptak, Vincent P.; Trutmann, Jeffrey A.; Zavala, Gregory H.

CORPORATE SOURCE: Dep. Chemistry, Loyola Univ. Chicago, Chicago, IL, 60625, USA

SOURCE: Synthetic Communications (1996), 26(10), 1943-1945

PUBLISHER: CODEN: SYNCVA; ISBN: 0039-7911

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:343745

AB A "one-pot" process for the preparation of a carotenoid synthon, EtOC(O)CMeCHO, has been developed that involves methoxide-promoted condensation of propionaldehyde with Me

formate, followed by exclusive O-alkylation of the resultant stabilized enolate, NaOCH<sub>2</sub>CH<sub>2</sub>CO.L73 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1996-1322 HCAPLUS Full-text

DOCUMENT NUMBER: 124:176588 Method of making 2,7-dimethyl-2,4,6-octatrieneal, a key intermediate in the commercial syntheses of various carotenoids

INVENTOR(S): Babler, James H.  
PATENT ASSIGNEE(S): Loyola University of Chicago, USA  
SOURCE: U.S., 9 PP.  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->PATENT NO. WO 1995-US13372 A1 19980617 AU 1995-39601 1995  
0108 <-->

## SN 10/564307 Page 9 of 139 STIC STN SEARCH 5/17/2007

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9412457	A1	19940609	WO 1993-US10276	1993 1027
JP 2002072251	A	20020312	JP 2001-160650	1991 0216
W: AU, CA, JP, KP, KR RM: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE		<--		
JP 2002100781	A	20020405	JP 2001-160671	1991 0216
JP 2003222838	A	20030808	JP 2002-331795	1991 0216
JP 3447730	B2	20030916	<--	
JP 2000292813	A	20001020	JP 2000-2212	1991 0327
JP 2000330139	A	20001130	JP <-- 2000-121941	1991 0327
JP 2001188257	A	20010710	JP <-- 2000-342919	1991 0327
JP 10213819	A	19980811	JP 1998-38120	1991 0511
JP 11233791	A	19990827	JP <-- 1998-323157	1991 0511
JP 2001144304	A	20010525	JP <-- 2000-304158	1991 0511
JP 2000004024	A	20000107	JP <-- 1999-153145	1992 0121
JP 3501977	B2	20040302	<--	
JP 2000031498	A	20000128	JP 1999-187097	1992 0121
JP 09166791	A	19970624	<-- 1996-294546	1992 0124
JP 05072564	A	19930326	JP <-- 1992-59403	1992 0213
		<--		

## SN 10/564307 Page 10 of 139 STIC STN SEARCH 5/17/2007

## US 5218464

	A	19930608	US 1992-836797	1992 0218
US 5349071	A	19940920	US <-- 1992-976219	1992 1125
AU 9456644	A	19940522	AU <-- 1994-56644	1993 1027
CN 1092758	A	19940928	CN <-- 1993-120597	1993 1124
US 5410094	A	19950425	US <-- 1994-255369	1994 0608
JP 09298331	A	19961112	JP <-- 1996-95713	1996 0417
JP 2552366	B2	19970910	<--	
JP 10041520	A	19980213	JP 1997-102689	1997 0404
JP 2090037	B2	19990510	<--	
JP 10223910	A	19980821	JP 1998-38121	1998 0204
JP 3057049	B2	20000526	<--	
JP 20203332	A	20020131	JP 2001-142474	2001 0511
JP 3380546	B2	20030224	<--	
JP 2004004890	A	20040108	JP 2003-168989	2003 0613
JP 3554663	B2	20040818	<--	
JP 2004006950	A	20040108	JP 2003-271415	2003 0707
JP 2004258681	A	20040916	JP <-- 2004-150976	2004 0520
JP 2004310123	A	20041104	JP <-- 2004-150975	2004 0520
JP 2004334224	A	20041125	JP <-- 2004-150974	2004 0520
PRIORITY APPLN. INFO.:			US <-- 1992-976219	A 1992 1125
			JP <-- 1991-77318	A1

SN 10/564307 Page 12 of 139 STC STN SEARCH 5/17/2007  
useful in the synthesis of vitamins (no data), are prepared by reacting carbonyl-containing compounds (e.g., cyclohexanone) with alkynes (e.g., 1-octyne) in the presence of strong bases (e.g., MeCO<sub>2</sub>K).

containing compounds (e.g., cyclohexanone) with alkynes (e.g., 1-octyne) in the presence of strong bases (e.g.,  $\text{Me}_3\text{COK}$ ).

L73 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1993-649580 HCAPLUS Full-text  
DOCUMENT NUMBER: 119-249580  
TITLE: Method of preparing C-18 ketones used in the  
preparation of vitamins E and K  
INVENTOR(S): Baber, James H.  
PATENT ASSIGNEE(S): Loyola University of Chicago, USA  
SOURCE: U.S., 13 pp.  
COPEN: USXXAM

```

<-- JP 2000-2212 A3 1991-0327
<-- JP 2000-342919 A3 1991-0327
<-- JP 1995-335554 A3 1991-0511
<-- JP 1998-38120 A3

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
PATENT NO. ----- KIND ----- DATE ----- APPLICATION NO. ----- DATE -----
US 5231232 A 19930727 US 1991-07462 1991
PRIORITY APPLN. INFO.: <-- US 1991-07462 1218 1991

```

<p style="text-align: right;">&lt;--</p> <p>JP 1998-38121 A3 1991 0511</p> <p>JP 1998-124729 A3 1992 0121</p> <p>JP 1999-153145 A3 1992 0121</p>	<p style="text-align: left;">1991 0511</p> <p style="text-align: right;">&lt;--</p> <p>CASREACT 119,249580 OTHER SOURCE(S): AB</p> <p>Methods for preparing unsatd. C-18 ketones which can be used in the synthesis of vitamins E and K1 are claimed. One procedure involves coupling a C-9 primary allylic halide to a carbonyl-group-containing C-9 terminal alkyne. A second, two-step procedure employs a C-4 bisallylic halide (molar excess) and a carbonyl-group-containing C-9 terminal alkyne to form a C-13 primary allylic halide. The C-13 primary allylic halide can then be converted to the desired C-18 ketone by reaction with 2-methyl-3-butyn-2-ol. Novel C-18 ketones (e.g., 14-hydroxy-6,14-dimethyl-10-methylen-5-pentadecene-7,12-diyne-2-one, C-13 allylic halides (e.g., 10-chloromethyl-6,10-undecadien-7-yn-2-one) and C-9 allylic halides (e.g., 6-chloromethyl-6-hepten-3-yn-2-ol) are formed in the process.</p>
	1218

JP 1992-34194		A3	1992	L73 ANSWER 11 OF 19	HCAPIUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1992-490545 HCAPIUS Full-text DOCUMENT NUMBER: 117-00345
				TITLE:	Method of making 2,7-dimethyl-2-octatrienylidene and derivatives
JP 1992-38637		A3	1992	INVENTOR(S): Babler, James H.	
			0129	SOURCE: Loyola University of Chicago, U.S., 9 P.	
JP 1992-187604		A3	1992	DOCUMENT TYPE: Patent	CODEN: USXKAM
			0622	LANGUAGE: English	
WO 1993-US10276	w	1993		FAMILY ACC. NUM. COUNT: 1	
		1027		PATENT INFORMATION:	
JP 2001-92845	A3	2001		PATENT NO.	KIND DATE APPLICATION
		0328		US 5107030	A 19920421 US 1991-6617
<--					
OTHER SOURCE(S): CASREACT 121:157133; MARPAT 121:157133					
AB Tertiary alkynols Me <sub>2</sub> CH(CH <sub>2</sub> ) <sub>3</sub> CHMe(CH <sub>2</sub> ) <sub>3</sub> C(CH <sub>2</sub> ) <sub>2</sub> CH <sub>2</sub> OR (OR = R = H, alkyl, alkenyl, alkoxyalkyl, trialkylsilyl, arylalkyl) (e.g., 1-(1-octynyl)cyclohexanol),					
WO 9215544		A1	19920917	WO 1992-US14	

**OTHER SOURCE(S):** CASREC 3211-157-33; MARPAT 121:157-153  
**AB** Tertiary alkynols Me<sub>2</sub>CH(C≡CH)<sub>n</sub> (R=M) (OR) Me (R = H, alkyl, alkenyl, alkoxalkyl, trialkylsilyl, aryalkyl) [e.g., 1-(1-octynyl)cyclohexanol],





**SN 10/564307 Page 17 of 139 STIC STN SEARCH 5/17/2007**

**REGISTRY MOLECULES OF INTEREST**

```

*>*> d his 14
L4      (FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
        1 S 123-35-3/RN
*> d 14 ide
L4      ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN      123-35-3 REGISTRY
ED      Entered STN: 16 Nov 1984
CN      1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)
OTHER NAMES:
CN      β-Geraniolene
CN      β-Mycrene
CN      2-Methyl-5-methylene-2,7-octadiene
CN      3-Methylcyclohexene-7-methyl-1,6-octadiene
CN      7-Methyl-3-methylene-1,6-octadiene
CN      Myrcene
CN      NSC 40264
DR      2151-31-3
MF      C10 H16
CI      COM
LC      STN Files: AGRICOLA, ANABSTR, BELLSTEIN*, BIOSIS, BIOPACNO, CA,
        CABAB, CAOLD, CAPUS, CASREACT, CHEMINFO, CHEMINTORIX, CHEMIST,
        CIN, CSChem, CSNB, DDERU, DETERM*, DRUGU, EMBASE, GMELIN*, HDB,
        IFICOB, IFRPAT, IFIUDB, IPA, MEDLINE, MRK*, MEDS-OHS, NAPRALERT,
        PIRA, PRMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULLDAT, USPATZ, USPATZL, USPATZL, USPATZL, USPATZL, USPATZL, USPATZL, USPATZL, USPATZL, VTB
Other Sources: DSII**, EINECS**, TSCA**
(*+Enter CHEMIST File for up-to-date regulatory information)

```



\*\* PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10169 REFERENCES IN FILE CA (1907 TO DATE)  
 51 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 10220 REFERENCES IN FILE CAPUS (1907 TO DATE)  
 89 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

\*> d his 16

L6 (FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
 1 S 1191-16-8/RN
\*> d 16 ide

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 1191-16-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-but-en-1-ol, 3-methyl-, acetate (6CI, 7CI, 8CI, 9CI)
OTHER NAMES:
CN γ,γ-Dimethylallyl acetate
CN 1-Acetoxy-3-methyl-2-butene
CN 3,3-Dimethylallyl acetate
CN 3-Betyl-1-acetoxyl-2-butene
CN 3-Betyl-1,2-butene-1-ol acetate
CN 3-Betyl-1,2-butene-1-ol acetate
CN Acetic acid 3-methyl-2-butenoate
CN Dimethylallyl acetate
CN Isopent-2-enyl acetate
CN Propenyl acetate
MF C7 H12 O2
CT COM
STN Files: AGRICOLA, ANABSTR, BELLSTEIN\*, BIOSIS, CA, CAOLD,
 CAPUS, CASREACT, CHEMINFO, CHEMIST, CIN, CSChem, CSNB, DDERU,
 IFICOB, IFRPAT, IFIUDB, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPATZ,

Other Sources: DSII\*\*, EINECS\*\*, TSCA\*\*
(\*+Enter CHEMIST File for up-to-date regulatory information)

**SN 10/564307 Page 18 of 139 STIC STN SEARCH 5/17/2007**





L28 43 SEA FILE-CASREACT ABB=ON PLU=ON PY<2004 OR PRY<2004 OR AY<2004 OR MY>2004 OR REVIEW/DT

L31 QUE ABB=ON PLU=ON PY<2004 OR PRY<2004 OR AY<2004 OR

L35 619 SEA FILE-HCAPLUS ABB=ON PLU=ON 14/RACT

L36 5337 SEA FILE-HCPLUS ABB=ON PLU=ON 15/BACT

L37 86 SEA FILE-HCPLUS ABB=ON PLU=ON 16/P

L38 347 SEA FILE-HCPLUS ABB=ON PLU=ON 17/P

L39 144 SEA FILE-HCPLUS ABB=ON PLU=ON 18/P

L40 0 SEA FILE-HCPLUS ABB=ON PLU=ON 136(L1,137)

L41 12 SEA FILE-HCPLUS ABB=ON PLU=ON L36 AND L37

L42 0 SEA FILE-HCPLUS ABB=ON PLU=ON L35 (1) (L38 OR L39)

L43 10 SEA FILE-HCPLUS ABB=ON PLU=ON L35 AND (L38 OR L39)

L44 20 SEA FILE-HCPLUS ABB=ON PLU=ON L40 OR L41 OR L42 OR

L45 143) 34945 SEA FILE-HCPLUS ABB=ON PLU=ON L9

L46 70 SEA FILE-HCPLUS ABB=ON PLU=ON (L35 OR L36) AND L45

L47 4036 SEA FILE-HCPLUS ABB=ON PLU=ON 19/RACT

L48 50 SEA FILE-HCPLUS ABB=ON PLU=ON (L35 OR L36) AND L47

L49 9 SEA FILE-HCPLUS ABB=ON PLU=ON L48 AND L44

L50 70 SEA FILE-HCPLUS ABB=ON PLU=ON L44 OR L46 OR (L48 OR

L49)

L52 47 SEA FILE-HCPLUS ABB=ON PLU=ON L51 AND L50

L53 QUE ABB=ON PLU=ON VITAMIN+E+PFT, OLD, NT/CT

L54 3 SEA FILE-HCPLUS ABB=ON PLU=ON L51 AND (L53 OR L54)

L55 1 QUE ABB=ON PLU=ON "DIETARY SUPPLEMENTS"+PFT, OLD, NT/C

L56 T QUE ABB=ON PLU=ON "FLAVORING MATERIALS"+PFT, OLD, NT/C

L57 T QUE ABB=ON PLU=ON "ODOR AND ODOROUS SUBSTANCES"+PFT,

L58 T QUE ABB=ON PLU=ON "OLD, NT/CT"

L59 45 SEA FILE-HCPLUS ABB=ON PLU=ON L52 AND L31

L60 43 SEA FILE-HCPLUS ABB=ON PLU=ON L28

L61 43 SEA FILE-HCPLUS ABB=ON PLU=ON L50 AND L31

L62 M: OR, SUPPLEMENT? OR FLAVOR?

L63 4 SEA FILE-HCPLUS ABB=ON PLU=ON L61 AND (L53 OR L56

L64 OR L57 OR L58)

L65 5 SEA FILE-HCPLUS ABB=ON PLU=ON L51 AND (L53 OR L56

L66 OR L57 OR L58)

L67 45 SEA FILE-HCPLUS ABB=ON PLU=ON L55 OR L59 OR L65

L68 6 SEA FILE-HCPLUS ABB=ON PLU=ON L66 AND L31

L69 13 SEA FILE-HCPLUS ABB=ON PLU=ON L63 OR L64

L70 17 SEA FILE-HCPLUS ABB=ON PLU=ON L65 OR L69

L71 43 SEA FILE-HCPLUS ABB=ON PLU=ON L67 NOT L70

>> dup rem 133 171  
FILE 'CASREACT' ENTERED AT 13:00:44 ON 16 MAY 2007  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'HEAPIUS' ENTERED AT 13:00:44 ON 16 MAY 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)  
PROCESSING COMPLETED FOR L33

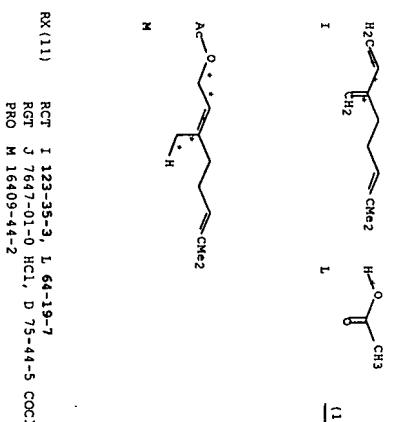
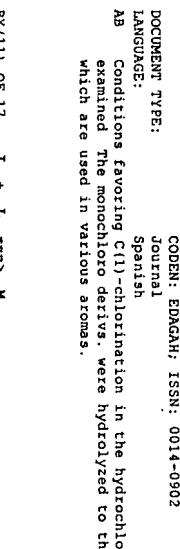
PROCESSING COMPLETED FOR L71  
67 DUP REM 133 L71 (1 DUPLICATE REMOVED)  
ANSWERS 1-25 FROM FILE CASREACT  
ANSWERS 26-67 FROM FILE HCPLUS

L74 67 DUP REM 133 L71 (1 DUPLICATE REMOVED)  
ANSWERS 1-25 FROM FILE CASREACT  
ANSWERS 26-67 FROM FILE HCPLUS

### STRUCTURE SEARCH RESULTS

L74 ANSWER 1 OF 67 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 116-6750 CASREACT Full-text  
TITLE: Hydrochlorination of myrcene. Selectivity for  
C1  
AUTHOR(S): De Bolard, Griselda V.; Cardell, Daniel; De  
Schiliuk, Irma G.  
CORPORATE SOURCE: Inst. Invest. Prod. Nat., IPNAYA, Sante Fe,  
3000, Argen.  
SOURCE: Essence, Derivati Agrumari (1990),  
60(3), 350-7

DOCUMENT TYPE: CODEN: EDGAAH; ISSN: 0014-0902  
LANGUAGE: Journal Spanish  
AB Conditions favoring C(1)-chlorination in the hydrochlorination of  $\beta$ -myrcene were examined. The monochloro deriva. were hydrolyzed to the alcs. (geraniol, nerol, etc.), which are used in various aromas.

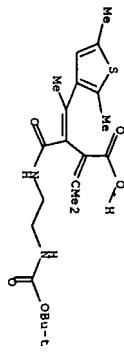


2003), (13), 2409-2417  
CODEN: EJOCFK; ISSN: 1434-193X  
Wiley-VCH Verlag GmbH & Co. KGaA  
Document Type: Journal  
Language: English

**SN 10/564307 Page 25 of 139 STIC STN SEARCH 5/17/2007**

**AB**

Functionalized fulgimides are regarded as a promising class of photochromic compds. for modulating the structure and function of biomols. A new synthetic route to fulgimides bearing amino-functionalized substituents at the imide N atom was developed. The synthesis of the fulgimides was achieved by base-catalyzed cyclization of phenacyl esters of the succinamic acids derived from fulgides and N-Boc-protected alkyl- and aryl-substituted diamines with triethylamine or tert-butyllithium. The UV-visible spectroscopic data and the photochromic properties of these new compds. were studied.



RX (2) OF 3 4 . . . C + D + 2 F ==> G +

H . . .  
YIELD 86% (40)

RX (2) RCT C 599164-65-5, D 599164-66-6, F  
70-11-1

STAGE(1)  
SOL 141-18-6, AcOEt

CON room temperature

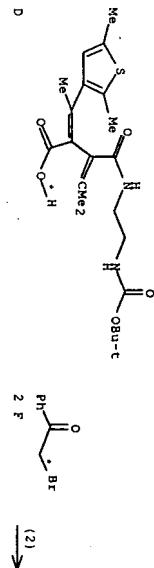
STAGE(2)

BGT 1 121-44-8

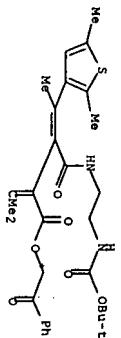
ET-3N

CON room temperature

REFERENCE PRO G 599164-67-7, H 599164-68-8  
COUNTER COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE  
TITLE: FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

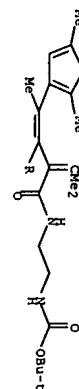


C



G  
YIELD 86% (60)

**SN 10/564307 Page 26 of 139 STIC STN SEARCH 5/17/2007**



H . . .  
YIELD 86% (40)

RX (2) RCT C 599164-65-5, D 599164-66-6, F  
70-11-1

STAGE(1)  
SOL 141-18-6, AcOEt

CON room temperature

STAGE(2)

BGT 1 121-44-8

ET-3N

CON room temperature

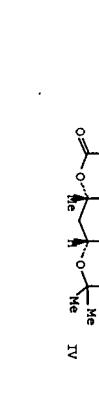
L74 ANSWER 3 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 139:117511 CASREACT Full-text  
TITLE: Biomimetic Synthesis of Fused Polyaryans:  
Oxacyclization Stereo- and Regioslectivity Is  
a Function of the Nucleophile

AUTHOR(S): Bravo, Fernando; McDonald, Frank E.; Neiwert,  
Wade A.; Do, Bao; Hardcastle, Kenneth I.  
CORPORATE SOURCE: Department of Chemistry, Emory University,  
Atlanta, GA, 30322, USA  
SOURCE: Organic Letters (2003), 5(12),  
2123-2126  
CODEN: ORLLET; ISSN: 1523-7060

PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



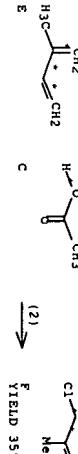
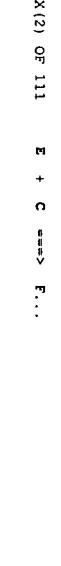
AB The stereoselectivity of Lewis acid-induced endo-regioselective oxacyclizations of 1,4-diepoxides is dependent upon the nature of the terminating nucleophile. For instance, ring-opening/recyclization of the carbamate-substituted diepoxyde I ( $R = \text{MeCO}$ ) provides a cis-fused bicyclic product II, whereas carbamate-derived I ( $R = \text{Me}_2\text{N}$ ) affords the trans-fused diastereomer of II. Stereoselective and regioselective conversion of the tertiary carbamate-terminated 1,4,7-triepoxyde III to tricyclic all-trans-fused polypyran IV is also demonstrated.



RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F

AUTHOR(S): Nanda, Ranji Rao, Palli, S.; Suryaprakash, R.; Lakshmi, V. V.; Acharyulu, P. V. N.; Murthy, Y. L. N.  
CORPORATE SOURCE: Dept. of Organic Chemistry, Andhra University, Visakhapatnam, India  
Chemistry (Rajkot, India) (2003), 14, 246-250  
SOURCE: CODEN: CIBRCI; ISSN: 0972-8376  
PUBLISHER: Trade Science Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

The title compds., (five new chromano isoxazoles) were synthesized by condensation of chalcones with hydroxylamine hydrochloride in the presence of alc. KOH. The synthesis involves four steps- Starting with the acylation of Resorcinol using anhydrous  $\text{ZnCl}_2$  and glacial acetic acid, which afforded Resacetophenone. Resacetophenone was then subjected to nuclear prenylation using isoprene in the presence of polyphosphoric acid and Xylene, to form 7-hydroxy-6-acetyl 2,2'-dimethyl chroman. Condensation of Chroman with various substituted benzaldehydes in the presence of alc. KOH furnished different chalcones. Finally, Chalcones were condensed with hydroxylamine hydrochloride in alkaline KOH medium and the title compds. were obtained. Compds. thus obtained were characterized by various spectroscopic techniques to confirm their structures.



RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F

STAGE(1)  
RCT B 50-7-40-4 t-Bu hypochlorite

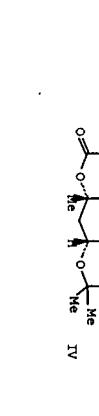
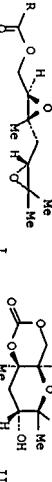
STAGE(2)  
RCT B 50-7-40-4 t-Bu hypochlorite  
SOL 64-19-7 AcOH  
CON 1 hour, room temperature

STAGE(2)  
RCT G 1310-73-2 NaOH  
SOL 7732-18-5 Water

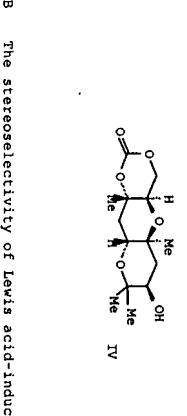
PRO F 24529-80-4  
NOTE stereoselective

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 4 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 141:350066 CASREACT Full-text  
TITLE: Synthesis and characterisation of new chromano isoxazoles



RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F



RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F

RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F

RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F

RX (12) OF 111    E + C ==> F...  
RX (13) OF 38 COMPOSED OF RX (1), RX (2)  
RX (13) A + B + E ==> F

STAGE(1)  
RCT B 50-7-40-4 t-Bu hypochlorite

STAGE(2)  
RCT B 50-7-40-4 t-Bu hypochlorite  
SOL 64-19-7 AcOH  
CON 1 hour, room temperature

STAGE(2)  
RCT G 1310-73-2 NaOH  
SOL 7732-18-5 Water

PRO F 24529-80-4  
NOTE stereoselective

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 4 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 141:350066 CASREACT Full-text  
TITLE: Synthesis and characterisation of new chromano isoxazoles

ACCESSION NUMBER:

137-140330

CASREACT

Full-text

Process for producing allyl halide compounds

DOI: 10.1442/137140330

Title: Process for producing allyl halide compounds

Boi, Noriyuki; Seko, Shinzo; Kimura, Kazutaka;

Takahashi, Toshiya

Japan

U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXXCO

Patent

Family Acc. Num. Count: 1

English

Priority Info:

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

PRO

SOL

RX(1)

RCT A 7B-73-5

RGT D 7726-95-6 Br2

PRO B 16526-19-5, C 16526-18-4

25154-42-1 Butane, chloro-

RX(2)

RCT B 16526-19-5, C 16526-18-4, F 546-89-4

PRO G 32659-14-6, H 32659-13-5

7732-18-5 Water, 6B-12-2 DMF

SOL

CN 2002-107071

2002-0205

JP 2001-10670

2001-0207

JP 2001-36572

2001-0214

JP 2001-349769

20011115

I74 ANSWER 6 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137-29505 CASREACT

Full-text

Palladium catalyzed oxidation of monoterpenes:

novel oxidation of myrcene with dioxygen

Goncalves, Jose Alton; Howarth, Oliver W.;

Gusevskaja, Elena V.

Departamento de Quimica, Universidade Federal

de Minas Gerais, Belo Horizonte, MG,

31270-901, Brazil

Journal of Molecular Catalysis A: Chemical (

2002), 185(1-2), 97-104

CODEN: JMCCEZ; ISSN: 1381-1169

Elsevier Science B.V.

Journal

Elsevier Science B.V.

English

G1

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

English

YIELD 67% (96)

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

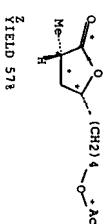
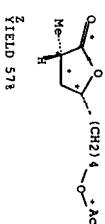
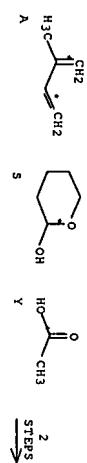
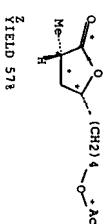
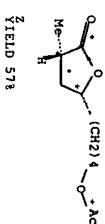
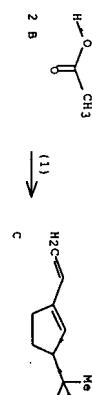
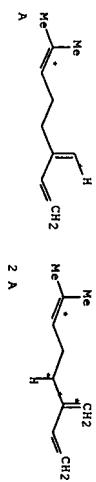
RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E

RX(1) OF 1 3 A + 2 B ==&gt; C + D + E



L74 ANSWER 7 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 136:15047 CASREACT Full-text  
 TITLE: Nickel-catalyzed homoallylation of aldehydes  
 AUTHOR(S): Kimura, Makamari; Eico, Akihiro; Tanaka,  
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of  
 Engineering, Nagasaki University, Nagasaki,  
 Shuji; Tamaru, Toshio  
 Ansgewandte Chemie, International Edition (2001), 40(19), 3602  
 CODEN: ACIEPS; ISSN: 1433-7821  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 LANGUAGE: English  
 AB Alddehydes and cyclic hemiacetals were efficiently homoallylated in presence of aqueous  
 Ni(acac)<sub>2</sub> and Et<sub>3</sub>B in THF. The reaction proceeded in reasonable yields with aqueous  
 glutaraldehyde.

RX(1) RCT A 123-35-3, B 64-19-7  
 RGT F 7782-44-7 02  
 PRO C 467449-32-7, D 467449-34-9, E 467449-33-8  
 CAT 7541-10-1 PGCl2, 7447-39-4 CUC12  
 SOL 64-19-7 AcOH  
 REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT

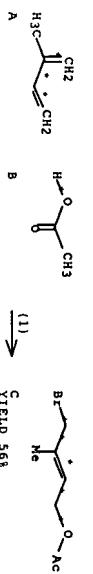
L74 ANSWER 7 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 136:15047 CASREACT Full-text  
 TITLE: New Syntheses of the Alkaloid Polonicumtoxin C  
 AUTHOR(S): Van, T. N.; De Kimpe, N.  
 CORPORATE SOURCE: Faculty of Agricultural and Applied Biological  
 Sciences, Department of Organic Chemistry,  
 Ghent University, Ghent, B-9000, Belg.  
 Tetrahedron (2000), 56(40), 7959-7973  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 LANGUAGE: English  
 AB Two new short syntheses of the alkaloid polonicumtoxin C were presented. In the first  
 pathway, polonicumtoxin C was obtained in two steps by alkylation of 6-methyl-2,3,4,5-tetrahydropyridine with (E)-4-bromo-3-methyl-1-(tetrahydro-2-pyanyl oxy)-2-butene and

RX(15) OF 18 COMPOSED OF RX(7), RX(11)

SN 10/564307 Page 33 of 139 STIC STN SEARCH 5/17/2007

subsequent deprotection of the THP group. In the second pathway, the cyclic ketimine was constructed via a short sequence of reactions involving first a sequential alkylation of the N-(isopropylidene)isopropylamine with N,N-disilyl-protected  $\alpha$ -bromopropylamine and (E)-4-bromo- $\alpha$ -methyl- $\beta$ -(tetrahydro-2-pyranoyloxy)-2-butene, then transimination and deprotection, with the latter two reactions occurring in one step.

RX(1) OF 28 A + B ==> C...



RX(1) RCT A 78-79-5, B 64-19-7

STAGE(1)  
RCT D 128-08-5 Bromosuccinimide

SOL 64-19-7 AcOH

STAGE(2)  
SOL 7732-18-5 Water

STAGE(3)  
SOL 75-09-2 CH2Cl2

PRO C 32659-14-6

NOTE: STEREOSELECTIVE

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L74 - ANSWER 9 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 130-325271 CASREACT Full-text

TITLE: Preparation of  $\beta$ -ocimene- $\gamma$  esters for use in perfumes and as aromatic substances

INVENTOR(S): Samburg, Horst; Sommer, Horst; Lambrecht, Stefan; Werner, Peter; Guentert, Matthias; Kindel, Gernot; Koppe, Volmar

PATENT ASSIGNEE(S): Haarmann und Reimer G.m.b.H., Germany

SOURCE: Ger. Offen., 14 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DE 19718774 A1 1990-05-06 DE 1971-19718774 19971105

EP 91579 A1 1990-05-12 EP 1998-120071 19981023

EP 91579 B1 2000-08-06

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,

ES 2207778 MC, PT, IE, SI, LT, LV, FI, RO T3 2004-06-01 ES 1998-120071 19981023

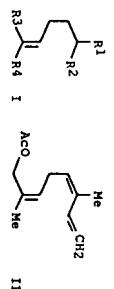
JP 11226350 A 1990-08-31 JP 1998-324452 19981030

JP 3583933 B2 2000-11-04 US 1998-186267 19981104

US 6034268 A 2000-03-07 US 1998-186267 19981104

SN 10/564307 Page 34 of 139 STIC STN SEARCH 5/17/2007

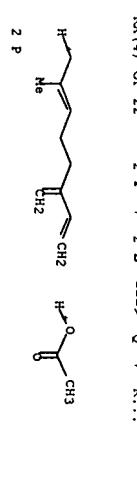
PRIORITY, APPN. INFO.: DE 1997-19718774 19971105  
OTHER SOURCE(S): MARPAT 130-325271 GI



RX(4) OF 22

2 P + 2 B ==> Q + R...

AB Compds. I (R1, R2 = Me, vinyl; R3, R4 = Me, CH2OCRS2; R5 = H, Cl-6-alkyl, C2-6-alkenyl) are useful as scents and aromatic substances. Thus, (3Z,6Z)-II was prepared from (E/Z)- $\beta$ -ocimene via chlorination with NaOCl solution followed by acetolysis with NaOAc in DMF containing NaI. (3Z,6Z)-II has a light fresh-green, fruity odor.



RX(4)

RCT P 123-35-3

STAGE(1)

RCT J 7601-52-9 NaOCl, K 64-19-7 AcOH  
SOL 7732-18-5 Water

STAGE(2)

RCT B 127-09-3  
RCT G 7601-82-5 NaI  
SOL 68-12-2 DMF

PRO Q 39228-41-0, R 99666-05-8

L74 ANSWER 10 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:  
129:43135TITLE:  
Diastereoselective aziridination of alkenesAUTHOR(S):  
Atkins, Robert S.; Ayscough, Andrew P.; Gattrell, W. T.; Rayman, Tony M.CORPORATE SOURCE:  
Dep. Chem., Univ. Leicester, LE1 7RH, UK  
Transactions 1: Organic and Bio-Organic Chemistry (1998), 17(1), 2783-2793  
CODEN: JCPB4; ISSN: 0300-922X  
Royal Society of ChemistryPUBLISHER:  
Royal Society of ChemistryLANGUAGE: English  
AB J-Amino-2-[(S)-1-hydroxy-2-(dimethylpropyl)quinazolin-4(3H)-one 9 (02NH) was prepared in four steps from (S)-tert-leucine in 43% yield without the need for chromatog. The corresponding 3-acetoxy-aminoquinazolinone, prepared in dichloromethane solution by reaction of 9 with lead tetracetate, reacts with alkenes in the presence of titanium(IV) tert-butoxide to give the corresponding aziridines stereoselectively. With styrene and butadiene the corresponding aziridines were obtained completely stereoselectively. Indane gave the expected endo-N-invertomer of aziridine as the kinetically-formed product (68%) also completely stereoselectively; equilibration to give a 1:1 ratio of exo-endo N-Invertomers occurs above 0°C. From an X-ray structure determination one aziridine product, the sense of diastereoselectivity in its formation is in agreement with the transition state model. Aziridinations of Me acrylate and of tert-Bu acrylate give the resp. products highly stereoselectively (d12>20:1) and with the same sense of diastereoselectivity as identified by an X-ray crystal structure determination previously. Aziridinations of  $\alpha$ -methylstyrene and Me methacrylate are less completely diastereoselective; isoprene reacts completely diastereoselectivity at its unsubstituted double bond but with little diastereoselectivity at its methyl-substituted double bond and the regioselectivity of aziridination on the two double bonds is 1:4:1 resp. by comparison to 1:4:7 in the absence of titanium(IV) tert-butoxide.

RX(108) OF 127 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13)  
 RX(108) 4 A + 4 B + 4 F + 4 N + 3 AG  
 ==> AH + AI + AJ + AK

**4 A**

**B**

**3 B**

**4 F**

**4 P**

**5**

**STEPS**

**1 1/4 Pb(IV)**

**2 AG**

**AG**

**PRO**

**G 215546-92-2**

**NTE**

**STEREOSELECTIVE**

**RX(1)**

**RCT**

**A 20859-02-3, B 64-19-7**

**STAGE(1)**

**SOL 7732-18-5 Water**

**PRO C 84621-74-9**

**NTE**

**STEREOSELECTIVE**

**RX(2)**

**RCT**

**C 84621-74-9**

**STAGE(2)**

**SOL 60-29-7 EtCO<sub>2</sub>**

**PRO**

**G 215546-92-2**

**NTE**

**STEREOSELECTIVE**

**RX(3)**

**RCT**

**G 215546-92-2**

**STAGE(1)**

**RGT L 302-01-2 N2H4**

**SOL**

**64-17-5 EtOH**

**STAGE(2)**

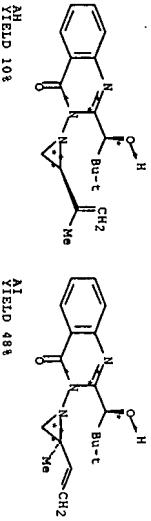
**SOL**

**7732-18-5 Water**

**PRO K 182160-10-7**

**NTE**

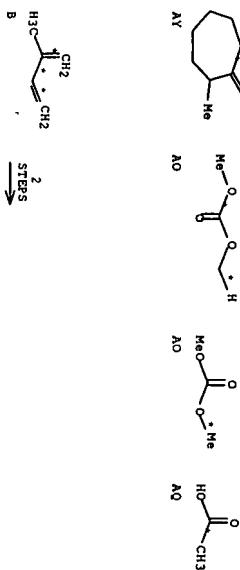
**STEREOSELECTIVE**



RX (4) RCT K 182160-10-7, N 546-67-8  
 PRO O 182160-08-3  
 SOL 865-49-6 CDCl<sub>3</sub>  
 NTE STEREOSELECTIVE

RX (13) RCT O 182160-08-3, AG 76-79-5  
 PRO AH 215546-97-7, AI 215546-96-6, AJ 215546-98-B, AK  
 SOL 215546-97-9  
 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 NTE STEREOSELECTIVE

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT



I74 ANSWER 11 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 127-277975 CASREACT Full-text  
 TITLE: Activated cyclooctenes are effective  
 dienophiles

AUTHOR(S): Liu, Hsing-Jang; Wang, Dan-Xiong; Kim, Jeung

Dep. of Chem., Univ. of Alberta, Edmonton, AB,  
 T6G 2G2, Can.

Canadian Journal of Chemistry (1997)

, 75(6), 899-912

CODEN: CJCHAG ISSN: 0008-4042

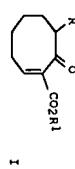
National Research Council of Canada  
 Journal  
 English

DOCUMENT TYPE:

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT

PRO

NOTE: STEREOSELECTIVE



AB

The first Diels-Alder addition of a diene to a cyclooctene dienophile has been observed. Three activated cyclooctene dienophiles (*i*; R = H, R<sub>1</sub> = Et; R = Me; R = Me, R<sub>1</sub> = Et) are studied with a variety of simple and functionalized dienes. Diels-Alder adducts are produced in excellent yields under very mild Lewis acid catalyzed conditions. The usual orientation rules are followed, and, as predicted, the products are formed, for the most part, exclusively by eserceno addition. The stereoselectivity is influenced by the substitution pattern of the diene in some cases. The factors influencing the stereochemistry, selectivity of the addition are discussed in some detail.

RX (24) RCT AX 932-56-9, AO 616-38-6

STAGE(1)  
 RCT AP 7646-69-7 NaH  
 SOL 110-71-4 (CH<sub>2</sub>COEt)<sub>2</sub>

STAGE(2)  
 RCT AO 64-19-7

STAGE(3)  
 RCT AP 7646-69-7 NaH  
 SOL 109-99-9 THF

STAGE(4)  
 RCT AR 5707-04-0 PhSeCl  
 SOL 109-99-9 THF

STAGE(5)  
 RCT E 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water, 60-29-7 Et<sub>2</sub>O

RX (39) OF 56 COMPOSED OF RX(24), RX(17),  
 RX (39) AY + 2 AO + AQ + B ---> AE

RX (17) RCT Y 196398-71-7

STAGE(1)  
 RCT D 7705-08-0 FeCl<sub>3</sub>

SOL 60-29-7 ER20

STAGE(2)

RCT B 78-79-5

STAGE(3)

RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

PRO AE 196398-86-4

REFERENCE COUNT: 24

THERE ARE 24 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L74 ANSWER 12 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 123142956 CASREACT Full-text

TITLE: Selective transformations of alkynols  
catalyzed by ruthenium complexes

AUTHOR(S): Bruneau, Christian; Kabouchi, Zahia; Neveux, Muriel; Seiller, Béatrice; Dineur, Pierre H.

CORPORATE SOURCE: Laboratoire de Chimie de Coordination

Organique, URA CIRB 415, Université de Rennes,

Campus de Beaulieu, Rennes, 35042, F-2.

Inorganica Chimica Acta (1994),

222(1-2), 155-63

CODEN: ICHAA3; ISSN: 0020-1693

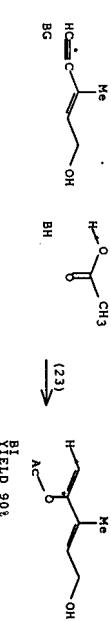
DOCUMENT TYPE: Journal

LANGUAGE: English

SOURCE: GI

AB Alkynols HC:tpbond:CHCOH, HC:tpbonds:CCMe:CHCl2OH react with carboxylic acids in the presence of  $[\text{Ru}(\mu\text{-OCH})(\text{CO})_2(\text{PPh}_3)]_{12}$  to selectively afford keto esters or trisubstituted hydroxy dienyl esters, depending on the possibility of effecting intramol. transesterification. The potential of  $\beta$ -oxopropiyl esters as mild acylating reagents and precursors of hydroxy amides, dipeptides, pseudodipeptides, polycarbonyl compds., and acetylenic 1,2-diols has been shown.

RX(23) OF 30 BG + BH ==&gt; BI



RX(23)

RCT BG 6153-06-6, BH 64-19-7

STAGE(1)

CAT 15156-73-3 Ruthenium tetracarbonylbis( $\mu$ -formato- $\kappa^2(\text{O}:\text{O}')$ )bis(triphenylphosphine).)di-, (Ru-Ru)  
SOL 108-88-3 PhMe

STAGE(2)

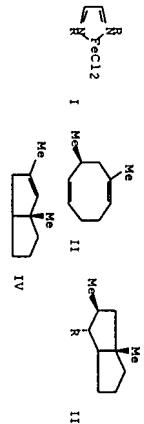
RCT D 144-55-8 NaHCO3

L74 ANSWER 13 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 116-214034 CASREACT Full-text  
TITLE: Enantioselective synthesis of cyclopentanoid compounds from isoprene and biperillene

Baldenius, Kai U.; Tom Dieck, Heindrik;  
Koenig, Wilfried A.; Ichlein, Detlef; Runge,  
Torsten  
Inst. Anorg. Angew. Chem., Univ. Hamburg,  
Hamburg, W-2000/13, Germany  
Angewandte Chemie (1992), 104(3),  
338-40 (See also Angew. Chem., Int. Ed. Engl.,  
1992, 31(3), 305-7)  
CODEN: ANEAD; ISSN: 0044-8249  
Journal German

CORPORATE SOURCE:  
SOURCE:  
AUTHOR(S):  
DOCUMENT TYPE: Journal

LANGUAGE: German  
GI



AB Cyclization of isoprene with piperylene in the presence of complex I [R = (1R)-menthyl] and butadiinemagnesium-2 THF gave 90% cyclooctadiene I, ee = 63%. Isomerization of II in the presence of an acid catalyst such as BF3-Et2O and an agent such as AcOH or PhH gave bicyclo compds. such as III (R = OAc, Ph) and IV.

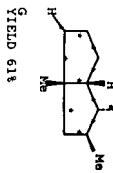
RX(5) OF 7 COMPOSED OF RX(1), RX(2)

RX(5) A + B + F ==&gt; G



RX(5)

A + B + F ==&gt; G



RX(1)

RCT A 78-79-5, B 2004-70-8  
PRO C 136541-38-5  
CAT 87226-76-6 Iron, dichloro[N,N'-1,2-ethanediyl]idenebis[5-methyl-2-(1-methylethyl)cyclohexaamidine]-N,N']<sup>-</sup>, [T-[IR-[1'1'R\*,2'S\*,5'R\*],B,5aI]]<sup>-</sup>, 83993-88-4 Magnesium, 2-buten-1,-diylisobutyrifuran)-, (T-4)-

NTE stereoselective

RX(2)

RCT C 136541-38-5, F 64-19-7  
RGT H 7664-83-9 H<sub>2</sub>SO<sub>4</sub>  
PRO G 136541-39-6  
SOL 64-19-7 AcOH  
NTE stereoselective

L74. ANSWER 14 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 116-20816 CASREACT Full-text  
TITLE: Pigments of fungi. XXI. Synthesis of

(±)-6-demethoxyaustracortinubin

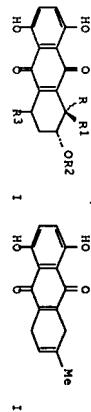
AUTHOR(S): Simon, Burns, Christopher J.; Gill, Melvyn; Saubern,

CORPORATE SOURCE: Sch. Chem., Univ. Melbourne, Parkville, 3052, Australia  
Australian Journal of Chemistry (1991)

DOCUMENT TYPE: CODEN: AUCHAS; ISSN: 0004-9425

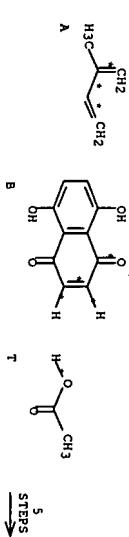
LANGUAGE: English

GI

AB 6-Demethoxyaustracortinubin (I, R-R<sub>2</sub> = H), is synthesized via the epoxide I (R<sub>2</sub> = bond, R<sub>1</sub>, R<sub>3</sub> = H) which is available in 73% yield over four steps from naphthalazarin.Hydrolysis of I (R<sub>2</sub> = bond, R<sub>1</sub>, R<sub>3</sub> = H) yields the diol I (R<sub>2</sub>, R<sub>3</sub> = H, R<sub>1</sub> = OH) which on hydrogenolysis affords 6-demethoxy-1-deoxyaustracortinubin (I, R-R<sub>3</sub> = H).Stereospecific benzylic hydroxylation of I (R-R<sub>2</sub> = H, R<sub>1</sub> = OH, R<sub>3</sub> = H) gives I (R-R<sub>2</sub> = H, R<sub>1</sub> = OH). Cleavage of I (R-R<sub>2</sub> = bond, R<sub>1</sub>, R<sub>3</sub> = H) with AcOH-AcJ gives I (R-R<sub>2</sub> = H, R<sub>1</sub> = OH).I (R = OAc, R<sub>1</sub>-R<sub>3</sub> = H; R = OH, R<sub>1</sub>, R<sub>3</sub> = H, R<sub>2</sub> = Ac; R = R<sub>2</sub> = R<sub>3</sub> = H, R<sub>1</sub> = OH), while methanolysis yields I (R = R<sub>2</sub> = R<sub>3</sub> = H, R<sub>1</sub> = OMe), and its isomer. Hydrogenolysis of I (R = R<sub>2</sub> = R<sub>3</sub> = H, R<sub>1</sub> = OAc, OMe; R = OH, R<sub>1</sub> = R<sub>3</sub> = H, R<sub>2</sub> = Ac) gives high yields of I(R-R<sub>3</sub> = H). Potentially more direct routes to I (R-R<sub>3</sub> = H) involving oxymercuration, epoxidation, and bromohydrin formation from the alkene II are not viable.

RX(55) OF 62 COMPOSED OF RX(1), RX(3), RX(10), RX(11), RX(12)

RX(55) A + B + T ==&gt; U



RX(1)

RCT A 78-79-5, B 475-38-7  
PRO C 14569-43-8

RCT C 14569-43-8  
RGT F 1310-71-2 NaOH  
PRO E 65698-32-0  
NTE H (+)

RX(10)

RCT E 65698-32-0  
RGT R 1493-13-6 F3CSO2H  
PRO M 137788-35-3

RX(11)

RCT M 137788-35-3  
RGT H 937-14-4 MCPBA  
PRO S 137788-36-4

RX(12)

RCT S 137788-36-4, T 64-19-7  
PRO U 137788-37-5

L74. ANSWER 15 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 111-194066 CASREACT Full-text  
TITLE: Acetoxyhalogenation of 1,3-diene hydrocarbons

AUTHOR(S): Ivanov, S. V.; Stadnikh, M. D. Leningr. Tekhnol. Inst., Leningrad, USSR

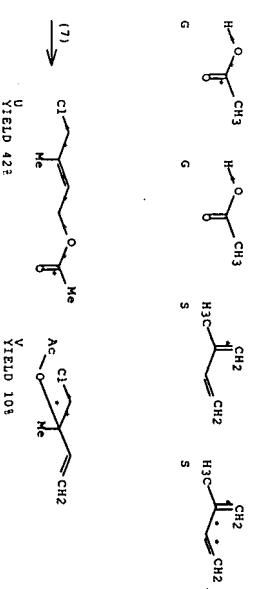
CORPORATE SOURCE: Zhurnal Obshchey Khimii (1989), 59(4), 865-73

DOCUMENT TYPE: CODEN: ZOKHA4; ISSN: 0044-460X  
Journal

LANGUAGE: Russian

Acyloxyclorination of divinyl with  $p$ -ClC<sub>6</sub>H<sub>4</sub>S(OCN)Cl<sub>2</sub> in HCO<sub>2</sub>H, AcOH, MeCl/2C<sub>2</sub>H<sub>5</sub>OAc led to the resp. 1,2- and 1,4-addition products ClOCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>R and ClCH<sub>2</sub>CH<sub>2</sub>(OCN)CH<sub>2</sub>CH<sub>2</sub> in comparable yields (i.e., 36:4 for R = H). LiClO<sub>4</sub> was found to suppress the competing polymerization reaction, and enhances the 1,4-addition reaction. Acyloxylolation of isoprene and CH<sub>2</sub>:CMeCMe:CH<sub>2</sub> was also studied. The authors warn of the possibility of explosion in the direct distillation of products from the reaction mixture, as well as the allergic nature of the reaction products.

RX (7) OF 14 2 G + 2 S ==&gt; U + V



RX (7) RCT G 64-19-7, S 78-79-5  
RGT E 17260-65-0 Benzene-sulfonamide, N,N,4-trichloro-, F  
PRO U 38872-49-0, V 24517-68-8  
SOL 64-19-7 ACOH

L74 ANSWER 15 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 112-36192 CASREACT Full-text

TITLE: Formal ene-chlorination of myrcene by

*N*-chlorosuccinimide

AUTHOR(S): Schulze, Klaus; Haute, Guenter; Koehler,

Guenther, Karl-Marx-Univ., Leipzig,

CORPORATE SOURCE: DDR-7010, Ger. Dem. Rep.

Zeitschrift fuer Chemie (1989),

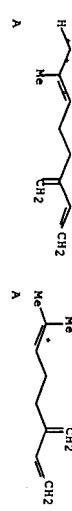
9(5), 167-8

DOCUMENT TYPE: JOURNAL

Journal

LANGUAGE: German  
AB Reaction of myrcene with NaSCN in ROH (R = H, Me, Ac) containing H<sub>2</sub>SO<sub>4</sub> gaveMe<sub>2</sub>CO(N)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)CH<sub>2</sub> in 64, 38, and 5% yields, resp., along with 21-57% CH<sub>2</sub>:CMeCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)CH<sub>2</sub> (1). It reacted with KSCN or NaOCl (R<sub>1</sub> = H, Ac, CHO) to give 44-80% CH<sub>2</sub>:CMeCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)CH<sub>2</sub> (R<sub>2</sub> = SCN, RN).

RX (4) OF 29 2 A + K ==&gt; L + C...



RX (4) RCT A 123-35-3, K 64-19-7  
RGT D 128-05-6 Chlorosuccinimide  
PRO L 124431-86-3, C 72420-53-2  
CAT 7664-93-9 H2SO4  
SOL 64-19-7 ACOH

L74 ANSWER 17 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 110-74799 CASREACT Full-text

TITLE: An efficient one-pot preparation of

2,4-pentadienoic esters from

 $\alpha,\beta$ -unsaturated aldehydes

AUTHOR(S): Rodriguez, J.; Waegell, B.

CORPORATE SOURCE: Fac. Sci., St-Jerome, Univ. Aix-Marseille III,

Marseille, F-13397, Fr.

Synthesis (1988), (7), 534-5

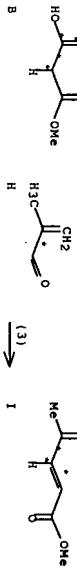
SOURCE: CODEN: SYNTHFR; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

AB  $\alpha,\beta$ -Unstd. aldehydes reacted with monoalkyl malonate and pyridine with a catalytic amount of DMAP in a regio- and stereoselective process to yield almost exclusively 2,4-pentadienoic esters with essentially (and in many cases exclusively) the 2E-stereoisomer. Thus, HO<sub>2</sub>CCCH<sub>2</sub>CO<sub>2</sub>Me and RCH:RC(=O) (R = H, Me, Ph, R<sub>1</sub> = H, R<sub>2</sub> = Me, RR<sub>1</sub> = CH<sub>2</sub>:CHO) gave 84-100% RCH:CHRICH:CHCO<sub>2</sub>Me.

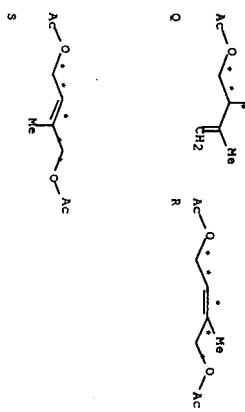
RX (3) OF 6 B + H ==&gt; I



L74 ANSWER 18 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 103:3870 CASREACT Full-text  
TITLE: Liquid-phase 1,4-diacetoxylation of conjugated  
dienes with tellurium(IV) oxide and alkali  
metal halides

AUTHOR(S): Demura, Sakae; Fukukawa, Shinichi; Patil,  
Suresh R.; Okano, Masaya  
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,  
Japan  
SOURCE: Journal of the Chemical Society, Perkin  
Transactions 1: Organic and Bio-Organic  
Chemistry (1972-1999) (1985), (3),  
499-503  
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Oxidation of  $\text{CH}_2:\text{CRCH}_2:\text{CH}_2$  ( $\text{R} = \text{H}$ ,  $\text{Me}$ ;  $\text{R}' = \text{H}$ ,  $\text{Me}$ ) with  $\text{TeO}_2$  in  $\text{HOAc}$   
containing  $\text{LiBr}$  gave isomeric mixts. of the corresponding dicetoxalkene 1,2- and 1,4-  
addition products; the product yields and selectivities were high in the presence of  
 $\text{excess LiBr}$ . The reaction also occurred in the presence of  $\text{NaBr}$ ,  $\text{KBr}$ ,  $\text{LiCl}$ ,  $\text{HBr}$ , or  
 $\text{iodine}$ , but yields and selectivities were lower. The mechanism is discussed.

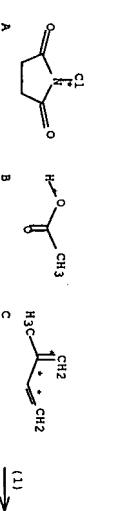


L74 ANSWER 19 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 98:142973 CASREACT Full-text  
TITLE: 4-chloro-3-methylcrotyl esters

PATENT ASSIGNEE(S): Dainippon Ink and Chemicals, Inc., Japan;  
Kawanura Physical and Chemical Research  
Institute  
SOURCE: Jpn. Kokai Tokyo Koho, 5 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO. RCT P 78-79-5, B 64-19-7, C 108-24-7  
JP 57183742 RCT G 7446-07-2 1e02, H 750-35-8 1eB  
PRO Q 30264-53-0, R 59055-00-4, S 59054-99-8

PRIORITY APPLN. INFO.: JP 19821112 19810501  
AB  $\text{RCO}_2\text{CH}_2\text{CH}_2:\text{CMeCH}_2\text{Cl}$  ( $\text{R} = \text{alkyl, aralkyl, Ph}$ ) were prepared by esterification of  $\text{RCO}_2\text{H}$   
with isoprene and chlorinating agents. Thus, 18 g  $\text{N}-\text{Chlorosuccinimide}$  was dissolved in 36  
g  $\text{HOAc}$  at 45°, 13 g isoprene in  $\text{HOAc}$  added at 45-55°, and the solution heated at 50-5°  
to give 4.5 g trans-1 ( $\text{R} = \text{Me}$ ) and 3.0 g  $\text{MeCO}_2\text{CH}_2\text{CH}_2:\text{CMeCH}_2\text{Cl}$ .





D

RX(1) RCT A 128-09-5, B 64-19-7, C 78-79-5  
PRO D 38872-49-0

L74 ANSWER 20 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 97-91789 CASREACT Full-text  
TITLE: Stereospecific palladium-catalyzed  
1,1-acetoxochlorination of 1,3-dienes

AUTHOR(S): Backvall, Jan E.; Nordberg, Ruth E.

CORPORATE SOURCE: Nyström, Jan E.; Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Sweden; Tetrahedron Letters (1982), 23(15), 1617-1620

SOURCE: CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: JOURNAL English

LANGUAGE: English  
GI



AB Pd-catalyzed oxidation of cyclic and acyclic 1,3-dienes in AcOH in the presence of LiCl/LiOAc gave 1-acetoxo-2-alkenes with high selectivity. E.g., addition of cyclohexa-1,3-diene to a mixture of benzoylone,  $Pd(OAc)_2$ , and LiCl/LiOAc in AcOH over 3 h, followed by reaction at room temperature for 5 h, gave 89% of a >98:2 mixture of cyclohexenes I ( $R = \alpha$ -Cl,  $R_1 = OAc$ ). The mechanism involves formation through (E)-acetoxypalladation of I double bond followed by external (E)-attack by Cl<sup>-</sup>. The 1,4-adducts were stereo- and regioselectively functionalized. E.g., substitution reaction of I ( $R = \beta$ -Cl,  $R_1 = OAc$ ) with Me<sub>2</sub>NH gave 93% I ( $R = \alpha$ -Me<sub>2</sub>N,  $R_1 = OAc$ ), which underwent substitution reaction with NaCH(CO<sub>2</sub>Me)<sub>2</sub> to give 80% I [ $R = \alpha$ -Me<sub>2</sub>N,  $R_1 = CH(CO_2Me)_2$ ].

RX(1) OF 19 A + B ==> C...  
L74 ANSWER 21 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 98-71124 CASREACT Full-text  
TITLE: Ruthenium-catalyzed Prins reaction  
Thivolle-Cazat, Jean; Tkatchenko, Igor  
Inst. Rech. Catal., Villeurbanne, 69626, Fr.

SOURCE: Communications (1982), 1(9), 1128-1132  
CODEN: JCCAT; ISSN: 0022-4936  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The preparation of 1,3-diol derivs. by the Prins reaction of dienes and alkenes with aldehydes and carboxylic acids was catalyzed by Ru salts. E.g., reaction of (H<sub>2</sub>C=CH)<sub>2</sub> with paraformaldehyde and MeCO<sub>2</sub>H in the presence of RuCl<sub>3</sub> in the absence of solvent for 20 h gave a 20:10 mixture of H<sub>2</sub>C=CH(OAc)CH<sub>2</sub>(CH<sub>2</sub>OAc)CH<sub>2</sub>NC<sub>2</sub>H<sub>5</sub> (III,  $R = H$ , Ac) together with 17 parts oligomeric H<sub>2</sub>C=CH(OAc)CH<sub>2</sub>(CH<sub>2</sub>OAc)CH<sub>2</sub>NC<sub>2</sub>H<sub>5</sub> (IV). The ratio of acyclic to oligomer varied with the reaction conditions. E.g., similar reaction in the presence of AcONa for 20 h gave a 2.5:39:6:24 mixture of II, III (R = H, Ac), and IV.

RX(1) OF 1 A + B + C ==> D  
PRO D 8018-03-2



RX(1) RCT A 78-79-5, B 50-00-0, C 64-19-7  
PRO D 8018-03-2

L74 ANSWER 22 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 97-145026 CASREACT Full-text  
TITLE: Synthesis of dithiobisbenzodihydrodienone and its related compounds from carboxylic acids and conjugated dienes  
AUTHOR(S): Fujita, Tatsunori; Watanabe, Shoji; Suga, Kyoichi; Miura, Toshiro; Sugahara, Kotaro; Kikuchi, Hajime; Dep. Appl. Chem., Chiba Univ., Chiba, 260, Japan  
CORPORATE SOURCE: Journal of Chemical Technology and Biotechnology (1979-1982) (1982), 32(3), 476-84  
SOURCE: CODEN: JCBDC; ISSN: 0142-0356

RX(1) RCT A 78-79-5, B 64-19-7  
PRO C 38872-49-0

SN 10/564307 Page 49 of 139 STIC STN SEARCH 5/17/2007

DOCUMENT TYPE:

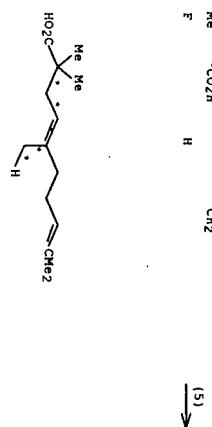
Journal

LANGUAGE:

English

AB Slow addition of isoprene in THF to 3-methylbutanoic acid, Me<sub>2</sub>CH-CH(Me)<sub>2</sub>, and Na naphthalide in THF under N at room temperature followed by refluxing 8 h and standing overnight gave 65% dihydrolavandulic acid (I), LiAlH<sub>4</sub> reduction of which gave 85% title compound Me<sub>2</sub>C-C(=O)CH<sub>2</sub>CH(CH<sub>2</sub>)-CHMe<sub>2</sub> (II). II is used in com. fragrances. Oxidation of II with pyridinium chlorochromate gave 81% dihydrolavandulyl aldehyde (III). Cyclization of I with H<sub>2</sub>S<sub>0</sub> in C<sub>6</sub>H<sub>6</sub> gave 82% 5,5-dimethyl-2-isopropyl-6-valero lactone (IV). Several analogs of I-IV were prepared similarly. 2-Alkyl- and 2,2-dialkyl-substituted 5-methyl-4-hexenols, 5-methyl-1-hexenals, and 5,5-dimethyl-5-pentanolides have sweet odors and can be used in perfumes.

RX (5) OF 103 F + H ==> I



RX (5) RCT F 79-31-2, H 123-35-3  
PRO I 10777-38-1

L74 ANSWER 23 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 96:139042 CASREACT Full-text  
TITLE: Selective 1,4-diacetoxylolation of conjugated

dienes with tellurium(IV) oxide

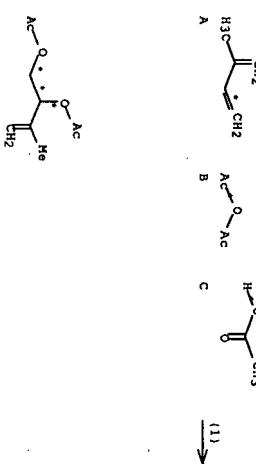
AUTHOR(S): Demura, Sakae; Miyoshi, Haruo; Tabata, Akira;

CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,

SOURCE: Japan  
Tetrahedron (1981), 37(2), 291-5  
CODEN: TETRAB; ISSN: 0040-4039

DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Conjugated dienes reacted with Ti(OAc)<sub>3</sub> in AcOH to give isomeric mixts. of the 1,2- and 1,4-diacetoxvalene addition products. 1,2-addition products predominated. E.g., CH<sub>2</sub>:OMC:CH<sub>2</sub> reacted with Ti(OAc)<sub>3</sub> (AcOH, 20°, 1 h) to give 71% of an 83:17 mixture of CH<sub>2</sub>:OMC(OAc)CHCOAc and AcOCH<sub>2</sub>OMC:CHCOAc. The mechanism of the reaction is discussed.

RX (1) RCT A 78-79-5, B 108-24-7, C 64-19-7  
RGT E 7446-07-3 TeO<sub>2</sub>, F 7550-35-8 LiBr  
PRO D 30264-53-0



L74 ANSWER 24 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 95:96978 CASREACT Full-text  
TITLE: Diacetoxylation of conjugated dienes with thallium(III) acetate in acetic acid

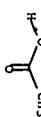
AUTHOR(S): Demura, Sakae; Miyoshi, Haruo; Tabata, Akira;

CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,

SOURCE: Japan  
Tetrahedron (1981), 37(2), 291-5  
CODEN: TETRAB; ISSN: 0040-4039

DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Conjugated dienes reacted with Ti(OAc)<sub>3</sub> in AcOH to give isomeric mixts. of the 1,2- and 1,4-diacetoxvalene addition products. 1,2-addition products predominated. E.g., CH<sub>2</sub>:OMC:CH<sub>2</sub> reacted with Ti(OAc)<sub>3</sub> (AcOH, 20°, 1 h) to give 71% of an 83:17 mixture of CH<sub>2</sub>:OMC(OAc)CHCOAc and AcOCH<sub>2</sub>OMC:CHCOAc. The mechanism of the reaction is discussed.

RX (6) OF 11 A + L + C ==> M  
A 1/3 Ti(III) L C (6) →



DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Oxidation of linear conjugated dienes with TiO<sub>2</sub> and LiBr in AcOH gave a mixture of 1,2- and 1,4-diacetoxvalenes. When the ratio of LiBr to TiO<sub>2</sub> was 5-10 the 1,4-isomer was produced highly selectively. E.g., reaction of 5 equiv butadiene with AcOH-Ac<sub>2</sub>O, 1 equiv TeO<sub>2</sub>, and 5 equiv LiBr at 125° for 20 h gave a 1:9 mixture of CH<sub>2</sub>:CHCH(OAc)CH<sub>2</sub>OAc and (E)- and (Z)-AcOCH<sub>2</sub>CH(OAc)CH<sub>2</sub>OAc.

RX (1) OF 6 A + B + C ==> D

SN 10/564307 Page 50 of 139 STIC STN SEARCH 5/17/2007

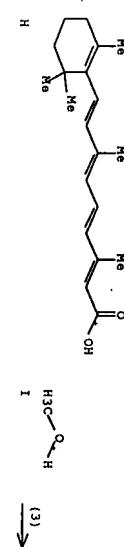
The diagram shows the chemical structure of a methyl acrylate monomer radical. It consists of a central carbon atom bonded to two methyl groups ( $\text{CH}_3$ ) and two carboxylate groups ( $\text{C}(=\text{O})\text{COO}^-$ ). A vertical line extends from the top carbon atom, representing the radical center.

RX (6) RCT A 2570-63-0, L 78-79-5, C 64-19-7  
PRO M 30264-53-0  
CAT 108-24-7 AC20

L74 ANSWER 25 OF 67 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 57-25494 CASREACT Full-text  
TITLE: Synthesis of carboxylic acid ester  
imidazole method  
AUTHOR(S): Staub, Heinz A.; Maunschreck, Alf  
CORPORATE SOURCE: Univ Heidelberg, Germany  
SOURCE: Chemische Berichte (1962), 95,

The basicatalyzed imidazole method allowed the preparation of esters from carboxylic acids and alcs., at room temperature in extremely short reaction periods with very good yields. The new method was applied to the prepn., or esters from highly unsat'd. alcs. and carboxylic acids as well as the vitamin A series and the prepn. of esters of tetr-alkes. Starting from  $N,N'$ -carbonyldimidazole (I), sym. and unsym. esters of carbonic acid were obtained, as well as imidazole-N-carboxylic acid esters, the pyrolysis of which yielded N-substituted imidazoles. Adipic acid dimidazole (12.31 g.), from equimolar amounts of adipic acid and I in tetrahydrofuran treated at room temperature with stirring with 6.2 N HCl, in 60 cc. absolute MeOH, the mixture treated after 0.5 min. with 17 cc. (CH<sub>2</sub>Cl<sub>2</sub>OEt<sub>2</sub>)<sub>2</sub>, b.p. 5-13 112.5°, m.p. 1.485. PhCH<sub>2</sub>OH (21.02 g.) in 70 cc. THF refluxed with 0.03 N Na, added at 20° to 33.73 g.  $N$ -Benzoylimidazole (II) in 60 cc. THF, evaporated after 1 h., the residue kept several hrs. with 80 cc. H<sub>2</sub>O and 80 cc. Et<sub>2</sub>O, and the extract worked up yielded 36.10 g. BrCH<sub>2</sub>Ph (III), m. 1950. b.p. 213 180-1. Na (0.20 g.) and 2.0 g. imidazole in 20 cc. THF refluxed, cooled, treated with Et<sub>2</sub>O yielded 7.35 g. PhCH<sub>2</sub>OH in 50 cc. THF, and processed in the usual manner yielded 34.1 g. III. 1 (27.88 g.) in 200 cc. THF stirred 2 h. at room temperature with 20.0 g. BrCH<sub>2</sub>OH and treated with a solution of 0.17 g. Na and 60.3 g. PhCH<sub>2</sub>OH in 80 cc. THF gave in the usual manner 30.7 g. III.  $N$ -Acetyl imidazole (16.75 g.) in 150 cc. THF mixed with 19.70 g. PhCH<sub>2</sub>OH treated at room temperature with a soln. of 0.40 g. Na and 4.0 g. imidazole in 50 cc. THF, kept overnight, evaporated, the residue shaken with the 3-fold amount of H<sub>2</sub>O, and extracted with Et<sub>2</sub>O yielded 20.25 g. PhCH<sub>2</sub>OH (20.15, 139-41.5, m.p. 1.5426). PhCH<sub>2</sub>OH in 30 cc. THF added at room temperature to 0.40 g. Na and 4.0 g. imidazole in 40 cc. THF, the mixture treated with 21.25 g. II in 30 cc. THF, kept overnight, and worked up gave 22.75 g. PhCH<sub>2</sub>OH (20.2, m. 39-3.5°, b.p. 1.137-8.5. 1 (19.89 g.) in 100 cc. THF stirred 2 h. with 14.30 g. BrCH<sub>2</sub>OH and treated at room temperature to 0.40 g. Na, 4.0 g. imidazole, and 15.71 g. PhCH<sub>2</sub>OH in 80 cc. THF, and worked up yielded 21.81 g. PhCH<sub>2</sub>OH (20.28, 12.80 g.) in 25 cc. THF, added at room temperature to 0.10 g. Na and 2.0 g. imidazole dissolved in 15 cc. THF, the mixture treated with 7.10 g.  $N$ -Pimeloylimidazole in 100 cc. THF, kept at room temperature overnight and some time later to 50%, evaporated, the residue ground with 250 cc. NaOH, kept hot, filtered, and the filtrate worked up yielded 16.49 g. C<sub>15</sub>H<sub>20</sub>NO<sub>2</sub> (215.31). PhCH<sub>2</sub>OH (14.08 g.) in 150 cc. THF stirred 1 h. with 16.20 g. I, treated with 0.46 g. Na in 5.0 g. MeOH, evaporated after 1 h., the residue shaken with 200 cc. H<sub>2</sub>O, and the aqueous solution extracted with Et<sub>2</sub>O yielded 11.05 g. PhCH<sub>2</sub>OH (20.2, m. 34-5.5°, b.p. 132.5-34°. Na (0.05 g.) and 1.0 g. imidazole in THF under N<sub>2</sub> treated successively with 2.20 g.  $N$ -Acetyl imidazole in 80 cc. THF and 2.93 g. vitamin A (IV) in 77 cc. THF stirred 2 h., evaporated, the residue kept with H<sub>2</sub>O overnight, extracted with Et<sub>2</sub>O, and the extract worked up yielded 2.17 g.

stirred 4 h. with 1.34 g. I, refluxed a few min., evaporated 45 cc. absolute MeOH under N<sub>2</sub>, treated with 0.18 g. Na in 15 cc. MeOH, kept overnight, filtered, evaporated, the residue shaken with 200 cc. H<sub>2</sub>O, and refrigerated overnight, yielded 2.25 g. Me ester of V, pale yellow needles, m. 55.5-6.5° [6.1 NH<sub>2</sub>-H2O]. V (55.5 g.) and 3.14 g. I processed in the usual manner, the residue dissolved in absolute EtOH, treated with 0.20 g. Na in 30 cc. EtOH, kept overnight, diluted with 150 cc. H<sub>2</sub>O. Shaken occasionally during 5 h. in vacuo, and extracted with petr. ether, and the extract worked up gave 5.37 g. Et ester of V, yellow oil, b.p. 60-61°. IV (31.2 g.) in 50 cc. THF treated with 0.05 g. Na and 1.0 g. imidazole, in 50 cc. THF, the mixture treated with 3.93 g. imidazole of V in 100 cc. THF, diluted after 5 h. with 80 cc. H<sub>2</sub>O, kept overnight, evaporated, and the residue extracted with 200 cc. petr. ether, yielded 4.62 g. IV ester of V, orange oil; all operations were conducted under N<sub>2</sub>. Ng. Palmitoyl-imidazole (4.57 g.) and 2.62 g. L-aspartic acid in 150 cc. H<sub>2</sub>O were kept overnight under N<sub>2</sub>, evaporated at 70° in vacuo, and recrystallized from MeCO yielded 1.23 g. 3-Palmitoyl-L-aspartic acid, m. 95-96°. Na (0.23 g.) dissolved in 30.0 g. Me3COH, cooled, added dropwise to 11.82 g. III, diluted with 50 cc. THF, kept overnight, evaporated, the residue kept 3 h. with 50 cc. H<sub>2</sub>O and 50 cc. EtCO<sub>2</sub>, and the EtCO<sub>2</sub> phase worked up yielded 10.38 g. MeCO<sub>2</sub> VIII, b.p. 9.9 52.5-53°, n<sub>D</sub><sup>20</sup> 1.4908. I (20.0 g.) in 40 cc. THF stirred 1 h. with 14.30 g. BzOH, mixed with 0.45 g. Na in 30.0 g. Me3COH, and worked up yielded 19.10 g. VI. Na(piper-*N*-butylbenzylimidazole)imide (9.87 g.) in 35 cc. Me3COH and 15 cc. THF added to 0.20 g. in 35 cc. Me3COH, kept at 33° overnight, diluted with 150 cc. H<sub>2</sub>O, stirred 4 h., evaporated, and extracted with EtCO<sub>2</sub> yielded 7.58 g. P-Me3C6H4CO2MeC<sub>6</sub>H<sub>3</sub>, b.p. 15.2-5.3°, n<sub>D</sub><sup>20</sup> 1.4904. Na (0.23 g.) in 23 cc. hot Me3COH cooled to 40°, treated with 18.76 g. isobutyric acid imidazole, kept overnight, distilled, the residue shaken with H<sub>2</sub>O, extracted with EtCO<sub>2</sub>, and the extract worked up yielded 13.6 g. iso-C<sub>10</sub>-CO2MeC<sub>6</sub>H<sub>3</sub>, b.p. 127.9°, n<sub>D</sub><sup>20</sup> 1.3928. Na (0.30 g.) in 30 cc. Me3COH and 25 cc. THF treated with 8.7 g. trimethylacetylimidazole in 10 cc. THF, kept overnight, distilled, and the residue worked up with H<sub>2</sub>O and EtCO<sub>2</sub> yielded 5.74 g. Me3CO2CH<sub>3</sub>, b. about 125°, n<sub>D</sub><sup>20</sup> 1.3935. N-Acetyl-imidazole (12.54 g.) in 140 cc. Me3COH, stirred 1 h., and filtered, yielded 12.0 g. to 2.28 g. Na in 184 cc. Me3COH, stirred 1 h., and filtered, yielded 7.0 g. Na dehydratate; an aqueous solution of the salt treated with cooling with concentrated H<sub>2</sub>O<sub>2</sub> yielded 30% dehydratetic acid, m. 108-10°. (aqueous EtOH). N-Propionyl-imidazole (12.0 g.) in 20 cc. THF treated with 0.23 g. Na in 16.5 g. Me3COH, kept 40 h. at 33°, neutralized with 100 cc. 0.1N HCl, and extracted with EtCO<sub>2</sub> yielded 5.45 g. (crude) EtCO<sub>2</sub>COMeC<sub>6</sub>H<sub>3</sub>, b.p. 92.5-4.5°, 1.4224, green with Fehling's in MeOH; a sample boiled with concentrated HCl in EtOH and treated with 2-(4-(ONI)<sub>2</sub>CH<sub>2</sub>HNHRH<sub>2</sub>) gave 2.4-(OZN)2CH<sub>2</sub>NNHRH<sub>2</sub>; CEC<sub>2</sub>, m. 152.5-4.5°. I (12.73 g.) in 20 cc. THF treated with 0.15 g. Na and 16.22 g. PHCO<sub>2</sub>H in 80 cc. THF, stirred 2.5 h., evaporated, and refrigerated yielded 9.9 g. CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>, m. 29.9-5°, n<sub>D</sub><sup>20</sup> 1.5551. Na (0.29 g.) in 28 cc. Me3COH and 10 cc. THF added dropwise during 2 h. to 21.18 g. I in 200 cc. THF, kept overnight, evaporated, diluted with H<sub>2</sub>O, and extracted with EtCO<sub>2</sub> yielded 15.9 g. N-carbo-tert-butoxymimidazole (VII), m. 45-7.5° (petr. ether). VII heated to 170° evolved CO<sub>2</sub>, the residue consisted of imidazole. Na (0.17 g.) in 19 cc. Me3COH added at 50° to 8.60 g. I in 22 cc. THF, kept overnight, refluxed 1 h., distilled, the residue treated with H<sub>2</sub>O, and refrigerated gave 4.65 g. CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>, m. 38.5-40.5°. (aqueous EtOH). Na (0.10 g.) in 2.4 cc. EtOH added to 0.8 g. VII in 0.8 cc. EtOH, kept at room temperature overnight, diluted with H<sub>2</sub>O, and extracted with EtCO<sub>2</sub> yielded 4.5 g. CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>, b. 139-41°, n<sub>D</sub><sup>20</sup> 1.3947. Na (0.13 g.) added slowly dropwise to 11.02 g. I in 170 cc. THF, heated 1.5 h. at 50°, evaporated, the residue kept 45 min. at room temperature with 200 cc. dry CCl<sub>4</sub>, filtered, and distilled gave 6.8 g. N-carboxymimidazole (VIII), b.p. 66-17° (9.7°, n<sub>D</sub><sup>20</sup> 1.4760). Imidazole with CICOEt also gave VII, b.p. 101.5-5.5°, n<sub>D</sub><sup>20</sup> 1.4763. PHCO<sub>2</sub>H (12.50 g.) containing 0.40 g. Na added dropwise to 19.7 g. I in 200 cc. THF, stirred 1 h. at 30°, evaporated, the residue kept some time at 20-30° in vacuo, diluted with 30 cc. dry CCl<sub>4</sub>, filtered, and the filtrate worked up gave 18.5 g. reddish oily N-carboxybenzoylimidazole (IX), n<sub>D</sub><sup>20</sup> 1.5416. Crude IX (6.28 g.) distilled in vacuo yielded 4.21 g. N-benzyloxy-imidazole (X), m. 70-2° (petr. ether). CICO<sub>2</sub>CH<sub>2</sub> (10.4-5 g.) and 8.34 g. imidazole heated 0.5 h. with stirring at 100° and diluted with 200 cc. dioxane precipitated 7.0 g. X, m. 69-70°. IV (11.33 g.) and 4.0 cc. EtOH heated 2 h. at 40-50°, kept overnight, diluted with 30 cc. H<sub>2</sub>O, and extracted after 2 h. with EtCO<sub>2</sub> yielded 5.96 g. EtCO<sub>2</sub>Bz<sub>2</sub>H<sub>2</sub>O (XI), b.p. 166-71, and 0.66 g. X, m. 69.5-72° (petr. ether). VIII (21.85 g.) and 16.84 g. PHCO<sub>2</sub>H in 20 cc. THF heated 3 h. at 80°, kept overnight, and worked up yielded 13.9 g. XI, b.p. 126-30°, n<sub>D</sub><sup>20</sup> 1.4933. Na (0.58 g.) in 13.50 g. PHCO<sub>2</sub>H and 20 cc. THF added to 19.45 g. VIII, kept overnight, and worked up in the usual manner yielded 9.1 g. XI, b.p. 129-33°, n<sub>D</sub><sup>20</sup> 1.4919, and 5.7 g. CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>, b.p. 205-7°. m. 21-3°.



H

RX (3)

RCT H 302-79-4, I 67-56-1  
 RGT F 530-62-1 Dimidazoyl ketone  
 PRO J 339-16-2  
 SOL 71-43-2 Benzene, 67-56-1 MeOH  
 NTE Classification: Esterification; Alkoxylation; #  
 Conditions: carbodiimidazole; benzene 4h; several mn Rf;  
 NaOMe MeOH; overnight/N2

REENTER DISPLAY FORMAT FOR ALL FILES (FILEDEFAULT):

&gt;&gt; d 174 26-67 ibib ed abs hitstr hitind

L74 ANSWER 26 OF 67 HCPLUS COPYRIGHT 2007 ACS on STN  
 DOCUMENT NUMBER: 2003-760441 HCPLUS Full-text

TITLE: Protocol for the development of the master

chemical mechanism, MCM v3 (part A); tropospheric degradation of non-aromatic volatile organic compounds

Saunders, S. M.; Jenkins, M. E.; Derwent, R.

G.; Pilling, M. J.  
 School of Chemistry, University of Leeds,  
 Leeds, LS2 9JT, UK

Atmospheric Chemistry and Physics (

SOURCE: 2003, 3(1), 161-180

CODE: ACPC; ISSN: 1680-7324  
 European Geophysical Society  
 Journal

LANGUAGE: English

ED Entered STM: 29 Sep 2003

AB Kinetic and mechanistic data relevant to the tropospheric degradation of volatile organic compounds (VOCs), and the production of secondary pollutants, were previously used to define a protocol which underpinned the construction of a near-explicit Master Chemical Mechanism. An update to the previous protocol is presented, which was used to

define degradation schemes for 107 nonaromatic VOCs as part of version 3 of the Master Chemical Mechanism (MCM v3). The treatment of 18 aromatic VOCs is described in a companion paper. The protocol is divided into subsections describing initiation reactions, the reactions of the radical intermediates and the further degradation of 1st and subsequent generation products. Emphasis is placed on updating the previous information, and outlining the methodol. which is specifically applicable to VOCs not considered previously (e.g., α- and β-pinene). The present protocol aims to take into consideration work available in the open literature up to the beginning of 2001, and some other studies known by the authors which were under review at the time. Application of MCM v3 in appropriate box models indicates that the representation of isoprene degradation provides a good description of the speciated distribution of oxygenated organic products observed in reported field studies where isoprene was the dominant emitted hydrocarbon, and that the α-pinene degradation chemical provides a good description of the time dependence of key gas phase species in α-pinene/NOx photooxidn. expns. carried out in the European Photoreactor (EUPHORE). Photochem. Ozone Creation Potentials (POCP) were calculated for the 106 non-aromatic non-methane VOCs in MCM v3 for idealized conditions appropriate to north-west Europe, using a phototchem. trajectory model. The POCP values provide a measure of the relative ozone forming abilities of the VOCs. Where applicable, the values are compared with those calculated with previous versions of the MCM.

Ozone Creation Potentials (POCP) were calculated for the 106 non-aromatic non-methane VOCs in MCM v3 for idealized conditions appropriate to north-west Europe, using a phototchem. trajectory model. The POCP values provide a measure of the relative ozone forming abilities of the VOCs. Where applicable, the values are compared with those calculated with previous versions of the MCM.

78-79-5, 2-Methylbuta-1,3-diene, reactions 79-20-9  
 , Methyl acetate 107-31-3, Methyl formate

, 109-60-4, n-Propyl acetate 133-86-4, n-butyl acetate 141-78-6, Ethyl acetate, reactions

540-88-5, tert-Butyl acetate  
 RI: FOJ (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)

(tropospheric degradation of non-aromatic volatile organic compds.)

RN 78-79-5 HCPLUS  
 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

RN 79-20-9 HCPLUS  
 Acetic acid, methyl ester (CA INDEX NAME)  
 CN H<sub>3</sub>C— $\overset{\text{O}}{\underset{\text{CH}_3}{\text{C}}} \text{—CH}_2$

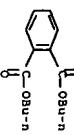
RN 107-31-3 HCPLUS  
 Formic acid, methyl ester (CA INDEX NAME)  
 CN  $\text{O}=\text{CH}_2 \text{—O—CH}_3$

RN 109-60-4 HCPLUS  
 Acetic acid, propyl ester (CA INDEX NAME)  
 CN  $\text{n-Pr—O—Ac}$

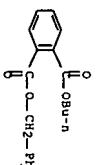
RN	123-86-4	HCAPLUS	
CN	Acetic acid, butyl ester	(CA INDEX NAME)	
n-Bu-O-Ac			
RN	141-78-5	HCAPLUS	
CN	Acetic acid ethyl ester	(CA INDEX NAME)	
Et-O-Ac			
RN	540-88-5	HCAPLUS	
CN	Acetic acid, 1,1-dimethylethyl ester	(CA INDEX NAME)	
t-Bu-O-Ac			
CC	59-2	(Air Pollution and Industrial Hygiene)	
IT	Section cross-reference(s): 53		
	50-00-0, Methanol, reactions	57-55-6, 1,2-Propanediol, reactions	
	60-29-7, Diethyl ether, reactions	64-17-5, Ethanol, reactions	
	61-18-6, Formic acid, reactions	64-19-7, Acetic acid, reactions	
	67-56-1, Methanol, reactions	67-63-0, Propan-2-ol, reactions	
	67-65-1, Propane, reactions	67-66-3, Trichloromethane, reactions	
	71-22-8, Propan-1-ol, reactions	71-36-3, Butan-1-ol, reactions	
	71-55-6, 1,1-Trichloroethane	74-84-0, Ethane, reactions	
	74-05-1, Ethene, reactions	74-86-2, Ethyne, reactions	
	74-87-3, Chloromethane, reactions	74-98-6, Propane, reactions	
	75-07-0, Ethanol, reactions	75-09-2, Propan-2-ol, reactions	
	75-20-5, Dichloromethane, reactions	75-65-0, 2-Methylpropane, reactions	
	75-85-4, 2-Methylpropan-2-ol	75-83-2, 2,2-Dimethylbutane, reactions	
	78-78-4, 2-Methylbutane-2-ol	75-97-8, 3,3-Dimethylbutan-2-one, reactions	
	78-87-5, 2-Methylbuta-1,3-diene,	78-92-2, Butan-2-ol, reactions	
	78-83-1, 2-Methylpropen-1-ol, reactions	78-93-3, Butanone, reactions	
	2-Methylpropanal	79-01-6, Trichloroethene, reactions	
	79-08-4, Propionic acid, reactions	79-20-9, Methyl glykoxal, reactions	
	79-29-8, 2,3-Dimethylbutane	80-66-8, Methyl acetate, reactions	
	96-14-0, 3-Methylpentane	96-22-0, Pentan-3-one, reactions	
	105-46-, sec-Butyl acetate	106-97-8, Butene, reactions	
	106-99-9, But-1-ene, reactions	106-99-0, Buta-1,3-diene, reactions	
	107-21-1, Ethane-1,2-diol, reactions	107-22-2, Ethyl formate, reactions	
	107-31-3, Methyl formate	107-83-5, 2-Methylpentane, reactions	
	107-87-9, Pentan-2-one	107-98-2, 1-Methoxypropan-2-ol, reactions	
	108-10-, 4-Methylpenten-2-one	108-20-3, Diisopropyl ether, reactions	
	108-93-0, Cyclohexanol, reactions	108-94-1, Cyclohexane, reactions	
	109-60-4, n-Propyl acetate	109-60-4, n-Propyl acetate, reactions	
	109-66-0, Pentane, reactions	109-67-1, Pentan-1-ene, reactions	
	109-87-5, Dimethoxymethane	110-54-3, Hexane, reactions	
	110-60-5, 2-Ethoxyethanol	110-60-5, Octane, reactions	
	110-82-7, Cyclohexane	111-65-9, Nonane, reactions	
	111-76-2, 2-Butoxyethanol	111-84-2, Nonane, reactions	
	115-07-1, Propene, reactions	115-10-6, Dimethyl ether, reactions	
	123-38-6, Propenal, reactions	123-42-2, 4-Hydroxy-4-methylpentan-2-one, reactions	
		123-51-3, (Reactant or reagent); RACT (Occurrence); RACT (Reactant); OCCU (Reactant or reagent); (Tropospheric degradation of non-aromatic volatile organic compds.)	
		REFERENCE COUNT: 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT	
L74	ANSWER 27 OF 67	HCAPLUS	COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:	2003-34833	HCAPLUS	FULL-TEXT
DOCUMENT NUMBER:	139189246		
TITLE:	Specification of volatile organic compound emissions for regional air quality modeling of particulate matter and ozone		
AUTHOR(S):	Malar, P. A.; Moran, M. D.; Scholtz, M. T.; Taylor, A.		
CORPORATE SOURCE:	Modelling and Integration Division, Air Quality Research Branch, Meteorological Service of Canada, Toronto, ON, Can.		
SOURCE:	Journal of Geophysical Research, [Atmospheres] (2003), 108(D2), ACH 21-ACH 2/51		
CODEN:	JGRD3; ISSN: 0148-0227		
PUBLISHER:	American Geophysical Union		
DOCUMENT TYPE:	Journal		
LANGUAGE:	English		
ED	Entered STN: 08 May 2003		
AB	A new classification scheme for speciation of organic compound emissions for use in air quality models is described. This scheme uses 81 organic compound classes to preserve net gas-phase reactivity and particulate matter (PM) formation potential. Chemical structure, vapor pressure, OH reactivity, f.p./b.p., and solubility data were used to create the 81 compound classes. Volatile, semi-volatile organic compounds are included. This classification scheme was used in conjunction with the Canadian Emissions Processing System (CEPS) to process 1990 gas- and particle-phase organic compound emissions data for summer and winter for a domain covering much of eastern North America. A simple post-processing model analyzed speciated organic emissions in terms of gas-phase reactivity and potential to form organic PM. Previously unresolved compound classes which may significantly affect O3 formation included biogenic high-reactivity esters and internal CG-8 alkene-als, and anthropogenic ethanol and propane. Organic radical production associated with anthropogenic organic compound emissions may be 20 orders of magnitude more important than biogenic-associated production in northern USA and Canadian cities, and a factor of 3 more important in southern US cities. Previously unresolved organic compound classes, e.g., low vapor pressure polycyclic aromatic hydrocarbons (PAH), anthropogenic diacids, dialkyl phthalates, and high C number alkanes, may have significant impact on organic particle formation. Primary organic particles (poorly characterized in national emissions databases) dominate total organic particle concns., followed by secondary formation and primary gas-particle partitioning. The effect of the assumed		

**SN 10/564307 Page 57 of 139 STIC STN SEARCH 5/17/2007**

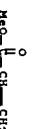
initial aerosol water concentration on subsequent thermodynamic, suggested hydrophobic and hydrophilic compds. may form external mists., and that sep. treatment for these groups may be required in future air quality model simulations. The post-processing model used overestimated organic particle formation relative to measurements, lacked the complexity of a regional air quality model and was not intended as an alternative to the latter. However, post-processing model results do provide guidance for treating organic gases and particles in future air quality modeling work. Future air quality model simulations should attempt to speciate primary particulate organic compds. and include more detailed organic compound classes. Future emissions profile measurements should specify gaseous high mol. mass organic compds. and primary orgs. emitted in particulate form (primary particle emissions are only available as a total particulate mass in currently available missions data).



RN 85-68-7 HCAPLUS  
CN 1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester (CA INDEX NAME)



RN 96-33-3 HCAPLUS  
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



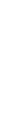
RN 105-37-3 HCAPLUS  
CN Propanoic acid, ethyl ester (CA INDEX NAME)



RN 106-65-0 HCAPLUS  
CN Butanoedioic acid, 1,4-dimethyl ester (CA INDEX NAME)



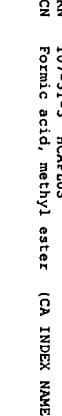
RN 107-31-3 HCAPLUS  
CN Formic acid, methyl ester (CA INDEX NAME)



RN 79-20-9 HCAPLUS  
CN Acetic acid, methyl ester (CA INDEX NAME)



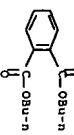
RN 80-62-6 HCAPLUS  
CN 2-Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



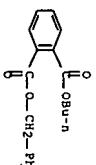
RN 84-74-2 HCAPLUS  
CN

**SN 10/564307 Page 58 of 139 STIC STN SEARCH 5/17/2007**

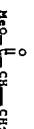
1,2-Benzenedicarboxylic acid, 1,2-dibutyl ester (CA INDEX NAME)



RN 85-68-7 HCAPLUS  
CN 1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester (CA INDEX NAME)



RN 96-33-3 HCAPLUS  
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



RN 105-37-3 HCAPLUS  
CN Propanoic acid, ethyl ester (CA INDEX NAME)



RN 106-65-0 HCAPLUS  
CN Butanoedioic acid, 1,4-dimethyl ester (CA INDEX NAME)



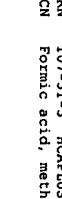
RN 107-31-3 HCAPLUS  
CN Formic acid, methyl ester (CA INDEX NAME)



RN 79-20-9 HCAPLUS  
CN Acetic acid, methyl ester (CA INDEX NAME)

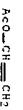


RN 80-62-6 HCAPLUS  
CN 2-Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



RN 84-74-2 HCAPLUS  
CN

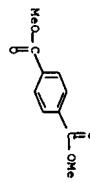
RN 108-05-4 HCAPLUS  
Acetic acid ethenyl ester (CA INDEX NAME)



RN 108-21-4 HCAPLUS  
Acetic acid, 1-methylethyl ester (CA INDEX NAME)



RN 109-60-4 HCAPLUS  
Acetic acid, propyl ester (CA INDEX NAME)



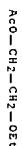
RN 110-19-0 HCAPLUS  
Acetic acid, 2-methylpropyl ester (CA INDEX NAME)



RN 111-15-9 HCAPLUS  
Ethanol, 2-ethoxy-, 1-acetate (CA INDEX NAME)



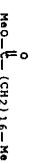
RN 111-82-0 HCAPLUS  
Dodecanoic acid, methyl ester (CA INDEX NAME)



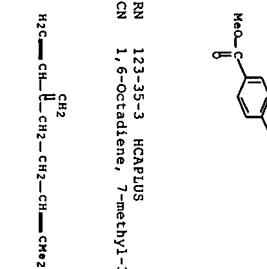
RN 112-39-0 HCAPLUS  
Hexadecanoic acid, methyl ester (CA INDEX NAME)



RN 112-61-8 HCAPLUS  
Octadecanoic acid, methyl ester (CA INDEX NAME)



RN 120-61-6 HCAPLUS  
1,4-Benzenediacrylic acid, 1,4-dimethyl ester (CA INDEX NAME)



RN 123-35-3 HCAPLUS  
1,6-Octadiene, 7-methyl-3-methylen- (CA INDEX NAME)



RN 123-66-0 HCAPLUS  
Hexanoic acid, ethyl ester (CA INDEX NAME)



RN 123-86-4 HCAPLUS  
Acetic acid, butyl ester (CA INDEX NAME)



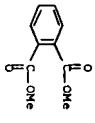
RN 124-10-7 HCAPLUS  
Tetradecanoic acid, methyl ester (CA INDEX NAME)



RN 131-11-3 HCAPLUS

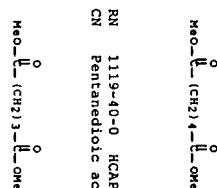
SN 10/564307 Page 61 of 139 STIC STN SEARCH 5/17/2007

SN 10/564307 Page 62 of 139 STIC STN SEARCH 5/17/2007



RN 136-60-7 HCAPLUS  
CN Benzoic acid, butyl ester (CA INDEX NAME)

RN 1119-40-0 HCAPLUS  
CN Pentanedioic acid, 1,5-dimethyl ester (CA INDEX NAME)



RN Ph-  
CN 140-98-5 HCAPLUS  
CN 2-Propenoic acid, ethyl ester (CA INDEX NAME)

RN 141-32-2 HCAPLUS  
CN 2-Propenoic acid, butyl ester (CA INDEX NAME)

RN 141-78-6 HCAPLUS  
CN Acetic acid ethyl ester (CA INDEX NAME)

RN 547-63-7 HCAPLUS  
CN Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)

RN MeO-  
CN EtO-  
CN Neo-  
CN 627-93-0 HCAPLUS  
CN Hexanedioic acid, 1,6-dimethyl ester (CA INDEX NAME)

CC 59-2 (Air Pollution and Industrial Hygiene)  
Section cross-reference(s): 53  
IT Aldehydes, reactions  
Alkanes, reactions  
Alkenes, reactions  
Alkynes, reactions  
Amines, reactions  
Carboxyl compounds (organic), reactions  
Epoxydes, reactions  
Ethers, reactions  
Hydrocarbons, reactions  
Ketones, reactions  
Naphthalene, reactions  
Naphthenic acids, reactions  
Petroleum spirits  
Polyalkylenes, reactions  
Polysiloxanes, reactions  
Terpenes, reactions  
Thiols, reactions  
Volatile organic compounds

RL: OCU (Occurrence); RACT (Reactant or reagent); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)  
(volatile organic compound emission speciation for modeling regional air quality and particulate matter and ozone formation)  
IT 50-00-0, Formaldehyde, reactions 50-32-8, Benz(a)aprene, reactions 53-70-3, Dibenz[*a*]anthracene 56-23-5, Carbon tetrachloride, reactions 56-55-3, Benz(a)anthracene 56-55-3D, Benzanthracene, alkyl derivs. 56-61-5, Glycerol, reactions 57-10-3, Palmitic acid, reactions 58-67-5, Propylene glycol, reactions 60-29-7, Ethylacetate, reactions 60-53-3, Aniline, reactions 64-17-5, Ethyl alcohol, reactions 64-18-6, Formic acid, reactions 64-19-7, Acetic acid, reactions 65-85-0, Benzoic acid, reactions 66-25-1, Hexanal 67-56-1, Methyl alcohol, reactions 67-63-0, Isopropylalcohol, reactions 68-12-2, Dimethyl formamide, reactions 71-23-8, n-Propylalcohol, reactions 71-36-3, n-Butylalcohol, reactions 71-41-0, Pentanol, reactions 71-13-2, Benzene, reactions 71-43-2D, Benzene, alky derivs. 71-55-6, 1,1,1-Trichloroethane 71-82-8, Methane, reactions 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 74-86-2, Acetylene, reactions 74-89-5, Methylamine, reactions 74-99-7, Methylenedibromide, Propane, reactions 74-99-7, Methylacetylene 75-00-3, Ethyl chloride 75-01-4, Vinyl chloride, reactions 75-04-7, Ethylamine, reactions 75-05-8, Acetonitrile, reactions 75-07-0, Acetaldehyde, reactions 75-08-1, Ethyl mercaptan

SN 10/564307 Page 64 of 139 STIC STN SEARCH 5/17/2007

110-63-4, 1,4-Butanediol, reactions 110-58-3, Hexane, reactions  
 110-3-0, Methylamyl ketone 110-58-3, Isobutanol, reactions  
 110-87-7, Cyclohexane, reactions 110-83-8, Cyclohexene,  
 110-86-1, Pyridine, reactions 111-15-9,  
 Cellobiose acetate 111-46-6, reactions 111-65-9, Octane,  
 reactions 111-66-0, 1-Octene 111-70-6, 1-Heptanol 111-76-2,  
 Butyl cellulose 111-77-3, Methylcarbitol 111-82-2,  
 Methyledecadanoate 111-84-2, Nonane 111-84-2, Nonane, Me  
 derivs. 111-87-5, Octanol, reactions 111-90-0, Caritol  
 112-27-6, Triethylamine glycol 112-30-1, Decanol 112-34-5,  
 Butyricarbital 112-39-0, Methylpalmitate 112-40-3,  
 Dodecanoate 112-41-4, 1-Dodecene 112-61-8, Methyl  
 stearate 112-95-6, Eicosane 115-01-1, Propene, reactions  
 115-10-6, Dimethylthiobuterol 115-11-7, Isobutylen, reactions  
 120-12-7, Anthracene, reactions 120-12-7D, Anthracene, alkyl  
 derivs. 120-12-7D, Anthracene, cyclopenten derivs.  
 120-61-6, Dimethylterephthalate 121-12-0, Triethylamine,  
 reactions 122-00-9, 1-(Chloromethyl)heptane 123-35-3, Myrcene  
 123-04-6, 3-(Chloromethyl)heptane 123-35-3, Myrcene  
 123-38-5, Propionaldehyde, reactions 123-42-2, Diacetone alcohol  
 123-51-3, Isooctylacetone 123-55-0, Ethylhexanone  
 123-72-8, Butyraldehyde 123-86-4, n-Butylacetate  
 124-04-9, Adipic acid, reactions 124-09-4, Hexamethylenediamine,  
 reactions 124-10-7, Methyl myristate 124-11-8,  
 1-Hexene 124-17-4, 124-18-5, Decane 124-18-5D, Decane, Me  
 derivs. 124-40-3, Dimethylamine, reactions 126-99-6,  
 Chloroprene 127-48-4, Perchloroethylene, reactions 127-91-3,  
**B-Pinene** 129-00-0, Pyrene, reactions 131-11-3,  
 Dimethyl phthalate  
**RL:** OCU (Occurrence, unclassified); RACT (Reactant or reagent); RCT  
**(Reactant):** OCCU (Occurrence); RACT (Reactant or reagent)  
**(volatile organic compound emission speciation for modeling regi-**  
**al air quality and particulate matter and ozone formation)**  
 131-08-8, Dipropenylphthalate 135-03-3, 1,2-Diethylbenzene  
 139-98-8, Sec-butylbenzene 136-60-7, Butylbenzoate  
 139-80-3, Limonene 140-66-9 140-88-5, Ethylacrylate  
 141-32-2, ButylAcrylate 141-43-5, Ethanolamine  
 reactions 141-78-6, Ethylacetate, reactions 141-93-5,  
 m-Diethylbenzene 142-22-0, Cyclopentene 142-82-5, Heptane,  
 reactions 142-96-1, Dimethyl ether 144-62-7, Oxalic heptate,  
 reactions 191-07-1, Coconene 191-24-2, Benzol(phi)perylene  
 191-26-4, Anthanthrene 192-97-2, Benzol(phi)pyrene 193-39-5,  
 Indeno[1,2,3-c]cdipyrene 195-19-9, Benzol(c)phenanthrene  
 196-78-1, Benzog[ol]chrysene 198-55-0, Perylene 203-12-3,  
 Benzo[ghi]fluoranthene 205-99-2, Benzo[kl]fluoranthene  
 206-49-0, Fluoranthene 207-08-9, Benzo(k)fluoranthene  
 208-96-8, Acenaphthylene 218-01-9, Chrysene 218-01-9D,  
 Chrysene, alkyl derivs. 224-41-9, Dibenzo[*l,j*]naphthalene  
 287-92-3, Cyclopentane 291-64-5, Cycloheptane 420-56-4,  
 Trimethylfluorosilane 463-49-0, Propadiene 463-55-1, Carbonyl  
 sulfide 463-82-1, 2,2-Dimethylpropane 475-38-7 488-33-3,  
 1,2,3,4-Tetramethylbenzene 496-10-6 496-11-7, Indane  
 496-17-0, Indan, alkyl derivs. 499-69-4, Camphorolene  
 500-00-5 502-42-1, Cycloneptane 503-17-3, 2-Butyne  
 504-60-9, Propiophene 505-57-7, 2-Tetenal 513-35-9,  
 2-Methyl-2-butene 546-73-8, 1,2,3-Trimethylbenzenes 529-20-4,  
 o-roluindihyde 535-77-3, 1-Methyl-3-isopropylbenzene 538-68-1,  
 p-tert-benzene 538-93-2, Isobutylbenzene 540-81-1,  
 Henry-benzene 540-81-1, Isobutylbenzene 540-81-1,  
 2,2,4-Trimethylpentane 541-05-9 541-73-1, m-Dichlorobenzene  
 544-73-3, Hexadecane 547-63-7, Methyl isobutyrate  
 555-02-2, Phellandrene 556-67-2,  
 Octamethylcyclotetrasiloxane 560-21-4, 2,3,3-Tri methylpentane  
 562-49-2, 3-Carboxy-1-pentene 563-45-1, 3-Methyl-1-butene  
 563-22-2, 2-Methyl-1-butene 563-70-6, 3-Carboxy-1-pentene  
 565-59-3, 2,3-Dimethylpentane 565-75-3, 2,3,4-Tri methylpentane

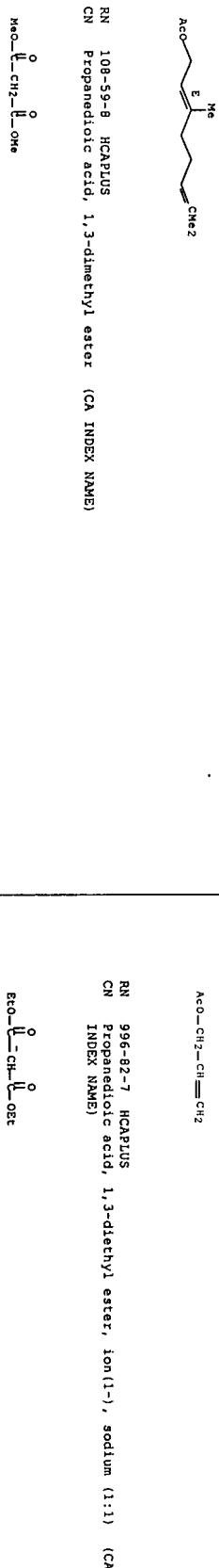
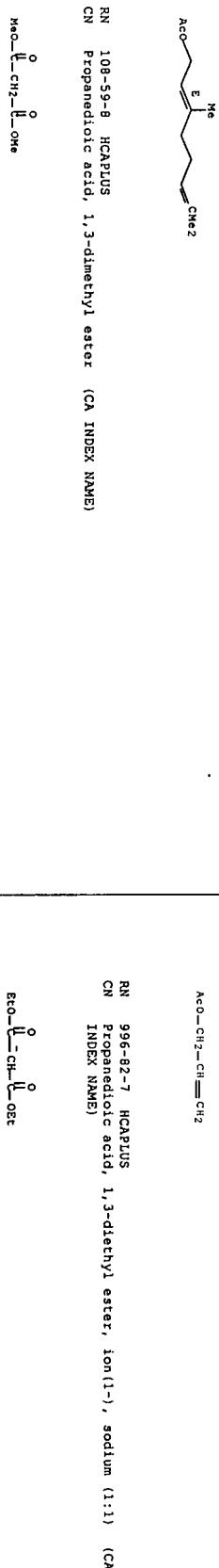
REFERENCE COUNT:

86 THERE ARE 86 CITED REFERENCES AVAILABLE

FOR THIS RECORD. ALL CITATIONS AVAILABLE

IN THE RE FORMAT

583-57-3 584-94-1, 2,3-Dimethylhexane 589-34-4, 3-Methylhexane  
 589-43-5, 2,4-Dimethylhexane 589-53-7, 4-Methylheptane  
 589-81-1, 3-Methylheptane 590-08-1, cis-2-Butene 590-19-2,  
 Methylallene 590-73-8, 2,2-Dimethylhexane 590-86-3,  
 Isovaleraldehyde 591-49-1, 1-Methylcyclohexene 591-56-4,  
 2-Methylheptane 591-78-6, Methylcyclopentene 592-41-6,  
 2,5-Dimethylhexane 592-27-8, 2-Methylheptane 592-41-6,  
 1-Hexene, reactions 592-43-6, 2-Hexene 592-46-7, 1-Hexene  
 592-78-9, 3-Heptene 593-45-3, Octadecane 598-01-6 610-38-8  
 611-14-3, 0-Ethyltoluene 616-12-6 619-99-8 620-14-4,  
 m-Ethyltoluene 624-29-3, cis-1,4-Dimethylcyclohexane 624-64-6  
 625-77-4, 2-Methyl-2-Pentene 625-79-4, Ethylisopropyl ether  
 627-20-3, cis-2-Pentene 627-93-0, Dimethylhexanedioate  
 627-97-4, 2-Methyl-2-Pentene 629-59-4, Tetradecane 629-62-9,  
 Pentadecane 629-78-7, Heptadecane 629-92-5, Nonadecane  
 629-94-7, Heneicosane 637-92-3, Ethyl-tert-butyl ether  
 644-35-9, 666-04-8, trans-2-Pentene 674-76-0,  
 4-Methyl-*t*-trans-2-Pentene 691-37-2, 4-Methyl-1-pentene  
 694-72-4, Octahydronaphthalene 696-99-7, 1-Ethoxy-1-cyclohexane  
 760-20-3, 3-Methyl-1-pentene 760-21-4, 2-Ethyl-1-butene  
 763-29-1, 2-Methyl-1-pentene 764-13-6 765-56-9,  
 4-Phenyl-1-butene 815-24-7  
 821-95-6, 1-Indene 872-05-9, 1-Decene 872-50-4, reactions  
 921-47-1, 922-02-3, 926-82-9, 3,5-Dimethylheptane 939-97-9  
 1002-43-3, 1004-21-1, 2-Butyltetrahydofuran 1068-87-7  
 1069-53-0, 2,3,5-Timethylhexane 1071-81-4 1074-43-7  
 1077-16-3, 1078-77-3, 1081-77-2 1119-40-0, Dimethyl  
 pentadeionate 1120-21-1, Undecene 1120-21-10, Undecene, Me-  
 derivative 1124-14-9 1319-75-3, Cresol 1320-16-7 1320-37-2,  
 Dichlorotetrafluorobutane 1321-60-4, Trimethylcyclohexanol  
 1321-90-4, Divinylbenzene, reactions 1321-94-4,  
 Methylnaphthalene 1322-20-9, Biphenyl 1333-49-9,  
 Dimethylcyclooctanol 1335-86-0, Methylcyclohexene 1502-39-1,  
 Methylcyclooctane 1560-06-1 1560-93-6 1560-97-0 1569-02-4,  
 1-Ethoxy-2-propanol 1634-04-9, Methyl-*t*-butyl ether  
 1636-39-1, Cyclopentylcyclopentene 1640-89-7, Ethylcyclopentene  
 1678-91-7, Ethylcyclohexene 1678-92-8, Propylcyclohexene  
 1678-93-9, Butylcyclohexene 1678-98-4 1795-16-0  
 1795-17-1, 1795-18-2, 1817-73-8 1820-39-5 2050-01-3, Isoamyl  
 isobutyrate 2051-30-1, 2,6-Dimethyloctane 2146-38-5,  
 Ethylcyclopentene 2198-23-4, 4-Nonenone 2213-23-2,  
 2,4-Dimethylheptane 2216-30-0, 2,5-Dimethylheptane 2216-32-2  
 2216-33-3, 3-Methyloctane 2216-34-4, 4-Ethyloctane 2719-92-0  
 2782-91-4, Tetramethylthiobutane 3074-71-3, 2,3-Dimethylheptane  
 3074-76-8, 3178-22-1, 3221-61-2, 2-Methyloctane 3406-61-3  
 304-65-7, 3522-94-9, 2,2,5-Timethylhexane 3775-51-2,  
 Isopropylcyclopentene 4032-94-6, 2,4-Dimethyloctane 4038-04-4  
 4050-45-7, trans-2-Hexene 4170-30-3, Crotonaldehyde 4222-15-5  
 4292-92-6, Pentylcyclohexane 4445-06-1 4830-99-3 4984-01-4  
 5364-81-0, Propenylcyclohexane 5505-41-5 5617-41-4  
 5989-27-5, D-Limonene 6006-33-3 6006-95-7 6434-78-2,  
 trans-2-Nonene 6703-81-7 6812-38-0 6842-15-5 6915-98-0,  
 2-Methyldecane 7146-60-3, 2,3-Dimethyloctane 7379-12-6,  
 2-Methyl-3-hexanone 7397-06-0, 1-Ethyl-Butyl-3,4-dimethylbenzene  
 7510-27-2, 7642-04-8, cis-2-Octene 7642-09-3, cis-3-Hexene  
 7688-21-3, cis-2-Hexene 8013-00-1, Terpinene 1057-37-5  
 1057-37-3, Pr-derivs. 12028-48-1, Trichlorobenzene  
 12408-10-5, Tetrachlorobenzene 13269-52-8, trans-3-Heptene  
 13466-78-9, 3-Carene 1450-23-8 14903-77-6 15869-22-8,  
 3,4-Dimethyloctane 15910-02-2, 15916-03-5 16747-26-5  
 18362-97-5, 19781-73-8, 20278-44-6, 2,4,5-Trimethylheptane  
 25154-55-3, Nonylphenol 25167-67-3, Butene 25265-71-8,  
 Diisopropylene glycol 25311-09-9, Diisopropyl benzene 25321-22-6,  
 Dichlorobenzene  
 (R): OCU (Occurrence, unclassified); (P): Pollutant; (R): Reactant  
 (Reactant); (OCU): (Occurrence); (R): Reactant or reagent)



$\text{AcO}-\text{CH}_2-\text{CH}=\text{CH}_2$

RN 10544-63-5 HCAPLUS  
2-Butenoic acid, ethyl ester (CA INDEX NAME)

Eto- $\ddot{\text{O}}-\text{CH}=\text{CH}-\text{CH}_2-\text{Me}$

IT

(Preparation and application of Palladium-allyl complexes)

IT 57-83-5, Progesterone, reactions 5222-0, Testosterone

IT 62-53-5, Aniline, reactions 64-19-7, Acetic acid, reactions

IT 65-85-0, Benzoic acid, reactions 67-56-1, Methanol, reactions

IT 67-63-0, Isopropanol, reactions 70-55-3, Tosylamide 74-85-1,

IT Etene, reactions 75-65-0, Oct-Butyl alcohol, reactions 75-77-4, Trimethylsilyl chloride, reactions 78-59-1, Isophorone

IT 78-79-5, 2-Methylbutadiene, reactions 78-88-6 78-94-4,

IT Methyl vinyl ketone, reactions 79-24-3, Nitroethane 85-11-6,

IT Phthalimide 90-39-1, (-)-Sparteine 96-33-3, Methyl

IT acrylate 97-94-9, Triethylborane 98-86-2, Acetophenone,

IT reactions 100-11-8, 4-Nitrobenzyl bromide 100-39-0, Benzyl

IT bromide 100-44-7, Benzyl chloride, reactions 100-51-6, Benzyl

IT alcohol, reactions 100-58-3, Phenylmagnesium bromide

IT 101-41-7, Methyl Phenylacetate 103-49-1, Diphenylamine

IT 103-54-8, Cinnamyl acetate 103-71-9, Phenyl isocyanate,

IT Methyl acetacetate 105-87-3, Geranyl acetate

IT 106-99-0, Butadiene, reactions 107-05-1, Allyl chloride

IT 107-13-1, Acrylonitrile, reactions 107-18-6, Allyl alcohol,

IT reactions 107-40-4, 2,4,4-Trimethyl-2-pentene 108-93-8

IT , Dimethyl malonate 108-94-1, Cyclohexanone, reactions

IT 108-95-2, Phenol, reactions 109-67-1, 1-Butene 109-99-7,

IT Diethylamine, reactions 110-83-8, Cyclohexene, reactions

IT 111-71-7, Heptanal 112-31-1, Decanal 115-11-1, Isobutene,

IT reactions 115-95-7, Linalyl acetate 122-39-4,

IT Diphenylamine, reactions 123-54-6, Acetylacetone, reactions

IT 124-11-0, Octanal 126-99-8, 2-Chlorobutadiene 140-29-4,

IT Phenylacetonitrile 140-88-5, Ethyl acrylate

IT 141-12-8, Naryl acetate 141-87-6, Ethyl

IT acetocetate 142-29-0, Cyclopentene 157-40-4, Spiropentane

IT 463-49-0, Allene 497-35-8, 2-Methylenorbornane 503-60-6

IT 513-81-5, 2,3-Dimethylbutadiene 532-31-0, Silver(I) benzoate

IT 543-63-5, Butyrmecubic chloride 554-61-0 563-47-3, Methylallyl

IT chloride 563-52-0, 3-Chloro-1-butene 563-63-3, Silver(I)

IT acetate 563-04-0, Allyl benzoate 590-18-1 591-49-1,

IT 1-Methylcyclohexene 591-87-7, Allyl acetate 591-93-5,

IT 1,4-Pentadiene 591-96-8, 1,3-Dimethylalane 591-91-9,

IT 2-Butenyl chloride 592-41-5, 1-Hexene, reactions 592-57-4,

IT 1,3-Cyclohexadiene 598-25-4, 1,1-Dimethylallene 601-57-0,

IT Cholesta-4-en-3-one 603-35-0, Triphenylphosphine, reactions

IT 603-35-0, Triphenylphosphine, reaction Product from palladium

IT dichloride dipe complex and DIBAL-H 609-02-5, Dimethyl

IT methylmalonate 614-20-0 614-47-1, (E)-Benzylideneacetophenone

IT 615-99-6, Diallyl oxalate 618-41-7, Phenylsulfonic acid

IT 623-43-8, 627-20-3, (Z)-2-Pentene 628-08-0, 2-Butenyl acetate

IT 629-20-9, Cyclococtatetraene 674-92-8, Dilute 689-06-5,

IT 4-Methyl-3-hexen-2-one 693-86-7, Vinylcyclopropane 693-99-0,

IT 1-Methylcyclopentene 754-03-2, Trimethylisilane 754-06-3,

IT Trimethyl(vinyl) stannane 762-12-1, Allyltrimethylsilane

IT 762-73-2, Allyltrimethylstannane 763-39-1, 2-Methyl-1-Pentene

IT 765-69-5, 2-Methyl-1,3-cyclopentanedione 829-55-5, Methylallyl

IT fumurate 820-71-3, Methylallyl acetate 824-79-3, Sodium

CC 29-0 (Organometallic and Organometalloidal Compounds)

IT 95-45-4, Dimethylglyoxime 116-17-6, Trisopropyl phosphite 546-89-4, Lithium acetate 624-44-9, Dimethyl fumarate 1067-52-3, Tributylmethoxystannane 2622-08-4,

IT

RN 10544-63-5 HCAPLUS

CN 2-Butenoic acid, ethyl ester (CA INDEX NAME)

IT

Meo- $\ddot{\text{O}}-\text{CH}=\text{CH}-\text{CH}_2-\text{Me}$

IT

RN 18424-76-5 HCAPLUS

CN Propanediol acid, dimethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)

IT

Meo- $\ddot{\text{O}}-\text{CH}=\text{CH}-\text{CH}_2-\text{one}$

IT

● Na+

IT

RN 123-35-3P,  $\beta$ -Myrcene

IT R1: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation and application of palladium-allyl complexes)

IT RN 123-35-3 HCAPLUS

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

IT

H<sub>2</sub>C=CH- $\ddot{\text{O}}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{Me}$

IT

R1: SPN (Synthetic Preparation); PREP (Preparation)

IT R2: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation and application of palladium-allyl complexes)

IT RN 123-35-3 HCAPLUS

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

P-toluenesulfinate 826-13-1 827-87-2 868-29-4 873-55-2, Sodium phenylsulfinate  
917-94-1D, Methylithium, reaction products with nickel tetracarbonyl 926-56-7, 4-Methyl-1,3-pentadiene 930-22-3,  
Vinlyloxirane 930-30-3 2-cyclopenten-1-one 934-56-5, 993-07-7,  
Trimethylphthalimide 960-16-7, Tributylphenylstannane 993-07-7,  
Trimethylisilane 996-82-7, Diethyl sodiomalonate  
1000-86-8, 2,4-Dimethyl-1,3-pentadiene 1075-25-9, Heptyllallene  
1074-82-4, Potassium phthalimide 1167-33-5 1184-88-9, Sodium  
pivalate 1189-09-9, Methyl (E)-geranate 1191-16-8  
3-Methyl-2-butenyl acetate 1192-37-6, Methylenecyclohexane  
1196-73-2 1205-42-1 1424-22-2 1450-4-2, Hexamethyldisilane  
1458-99-7, 4-Chloropent-2-ene 1461-29-9, Tributylchlorostannane  
1469-70-1, Allyl ethyl carbonate 1489-55-2 2-Methyl-1,3-  
Cyclohexadiene 1521-51-3, 3-Propenylcyclohexene 1528-30-9,  
Methyleneencyclopentane 1541-29-3 1578-96-3 1617-18-1, Ethyl  
3-butenoate 1617-19-2, Ethyl 3-methyl-3-butenoate 1700-10-3,  
1,3-Cyclooctadiene 1746-13-0, Allyl phenyl ether 1809-67-2  
1896-62-4 2001-45-8, Tetraphenylphosphonium chloride  
2004-70-8, (E)-1,3-Pentadiene 2227-97-1, 1-Phenyl-1,2-Pentadiene  
2277-99-3, Phenylalane 2384-90-9, Butylallene 2442-10-6  
2483-57-0, Methyl nitroacetate  
ketone 3618-12-0, Cyclooctene 3766-70-1, Geranylacetone  
4054-38-0, 1,3-Cycloheptadiene 4074-22-0, Diacetone  
cyclohexadiene 4093-64-1, Tosyl isocyanate 4112-09-8  
2783-10-0, 5-Methylhexa-1,3-diene 2923-17-3, lithium  
trifluoroacetate 3066-75-9, Allyl diethyl phosphate 3282-12-4, Phenyl diazomethyl  
(E)-Hexa-1,3-heptene 4431-24-7, 1,2-Bis(diphenylarmino)ethane  
4485-16-9, 4-Methyl-1,3-heptene 4497-92-1, (+)-2-Carene  
4653-22-3, 4-(2,6-dimethyl-3,5-di-  
4736-61-2, (Z)-3-Methoxy-19-norpregna-1,3(5),10,17(20)-tetraene  
4883-67-4, 2-Nitrocyclohexanone 4894-61-5, (E)-1-Chlorobut-2-ene  
4984-03-8, (E)-1-(Trimethylsilyl)prop-1-ene 5194-50-3,  
(E,Z)-Hexa-2,4-diene 5194-51-4, (E,E)-Hexa-2,4-diene  
5289-87-7, Geranyl chloride 5395-20-0, Benzyl p-tolyl sulfone  
5453-93-0 5489-14-5, Silver(I) propanoate 5674-01-1,  
2-Methylallylmagnesium chloride 5702-13-8  
2-Methylallylmagnesium chloride 6108-61-8, (Z,Z)-Hexa-2,4-diene  
6117-91-5, 2-Buten-1-ol 6142-73-0, Methylenecyclopropane  
6279-86-3 6290-45-7, N,N-Bis[(tert-butoxycarbonylmethyl)]amine  
6366-84-2 6651-36-1 6690-12-6, 9-Oxabicyclo[6.1.0]non-2-ene  
6705-51-7, 7-Oxabicyclo[4.1.0]hept-2-ene 6737-11-7 6790-37-0,  
4-Epoxy-1-pentene 6790-38-1, Allylloxirane 6921-34-2,  
Benzylmagnesium chloride 7129-41-1, 6-Oxabicyclo[3.1.0]hex-2-ene  
7129-41-1, 6-Oxabicyclo[3.1.0]hex-2-ene  
7217-11-2 7299-28-7, Tributyltin trifluoroacetate  
7422-28-8 7437-61-8 7770-41-4 1054-63-5, Ethyl  
2-butenoate 12077-82-6, Bis[(η<sup>5</sup>-allyl-allyl)]μ-bromopalladium]  
12081-43-5, Bis[(η<sup>3</sup>-bromo(η<sup>3</sup>-2-butenyl))palladium]  
13103-4-1 13118-25-5 13211-09-1 13463-19-3D, Nickel  
tetracarbonyl, reaction products and methyltin or  
benzylmagnesium chloride 1346-18-9, 3-Correne 13905-0-7,  
5-Methyl-1,4-hexen-3-one 14155-7-2, Allylmercury chloride  
14219-90-0, Thallium acetoximate 14371-10-9  
1483-67-1, tert-Buyl (trimethylsilyl) sulfide 14582-56-4,  
Bis(acetonitrile)dichloropalladium 14750-79-9 15022-08-9,  
Diethyl carbamate 1522-48-5, Dilithium tetrachloropalladate  
16510-49-9, 1,2,3-Triphenylcyclopropene 16712-86-8,  
Δ<sup>4</sup>-Cholestan-17-one 16733-97-4, Cyclopentadienyl lithium  
17094-21-2 17318-89-1, 1,2-Dimethyl-1,4-cyclohexadiene  
17422-12-7 17447-60-8 17651-97-7 18024-77-4,  
1,1-Trichloro-2,2,2-trimethylsilane 18424-76-5,

Dimethyl sodiomalonate 18522-02-4 18709-01-8  
RL: RCF (Reactant); RACR (Reactant or reagent)

'Preparation and application of palladium(allyl) complexes)

IT 100-52-7P, Benzaldehyde, preparation 123-35-3P,

β-Mercapto-2-Cyclohexen-1-one 1121-18-2P,

2-Methyl-2-Cyclohexen-1-one 31312-87-6P, Allyl P-tolyl sulfone

3724-55-8P, Methyl 3-butenoate 12081-18-IP, Bis[ $\mu$ -chloro(η<sup>3</sup>-2-methylallyl)palladium] 12081-22-0P,

Bis[η<sup>3</sup>-2-butenyl(μ-chloro)palladium] 1447-34-6P

16939-57-4P, (E)-1-Phenyl-1,3-butadiene 20657-21-0P

24931-66-6P, 2-Butenyl P-tolyl sulfone 33307-86-6P

33306-45-5P, 35988-93-1P, Tributyl(E)-but-2-enylstannane

53799-96-1P, 53799-97-2P 55820-06-9P

55833-94-8P 7616-46-6P

7773-11-6P 7794-71-8P

87567-12-2P

88076-44-2P 9143-64-7P 95177-50-0P

100898-93-9P 6589-37-6P

RL: RCF (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

IT Preparation and application of palladium-allyl complexes)

94-66-6P 104-55-2P, Cinnamaldehyde 111-13-7P, Hexyl methyl

ketone 122-57-6P 502-61-4P, (3E,6E)- $\alpha$ -Farnesene

601-1-6P, 5α-Cholest-1-en-3-one 601-55-8P,

5α-Cholest-1-en-3-one 818-58-6P 877-94-1P,

S-Pheylpent-4-en-2-one 934-10-1P 935-00-2P

936-67-4P, 2-Methylallylcyclohexanone 1002-35-3P, 1,3-Octatriene

1117-65-3P 1120-73-6P, 2-Methylcyclopent-2-en-1-one 1123-34-8P

1205-84-1P, (E)-Ethyl 4-phenyl-3-butenoate 1208-44-2P

1271-03-0P, (η<sup>3</sup>-Allyl)(η<sup>3</sup>-cyclopentadienyl)palladium

1489-50-5P, 2-Methylencyclopentan-1-one 1516-84-0P

1674-03-4P, trans-Pinocervol 1754-62-7P 2436-90-0P

2499-22-0P, 2609-23-6P 3045-98-5P 3318-55-4P

3393-45-1P 3912-67-7P 3491-27-8P 3664-60-6P, 7-Octen-2-one

3710-30-3P, 1,7-Octadiene 3798-61-1P 4005-80-9P

3-Cyclohexen-1-one 4117-81-9P 4734-90-1P, 3-Cycloocten-1-one

5428-09-1P 5558-87-2P 5629-57-2P 5666-17-1P 6032-63-7P

6610-21-5P, 6-Methylencyclopentan-1-one 6728-26-3P

(E)-Hex-2-enal 1063-05-6P 7688-51-9P 10006-38-9P

10281-55-2P 10281-56-2P 10428-56-3P 10491-63-1P

10500-10-1P 10500-11-5P 5-Pheylpent-3-en-2-one

12012-87-2P, Bis[(η<sup>4</sup>-chloro)(η<sup>3</sup>-2-chloroallyl)palladium]

12080-38-1P 12084-71-0P, Bis[( $\alpha$ -acetetoibis(η<sup>3</sup>-

allyl)]palladium 12090-09-4P 12090-59-6P

12097-84-6P, (η<sup>3</sup>-Allyl)chlorotriphenylphosphine)palladium

12099-33-1P 12111-01-1P 12128-99-6P 12131-44-1P

Bis[(η<sup>4</sup>-chloro)(η<sup>3</sup>-2-butenyl)palladium]

12115-45-3P 1215-16-4P 12156-09-1P 12182-66-2P 12240-87-8P,

12245-05-5P 12245-51-1P 12245-52-2P

12245-53-3P 1225-70-4P 12246-02-5P 12281-94-6P

12288-41-1P 12302-54-8P 12308-56-4P

12309-85-2P 13295-90-4P 13891-96-8P, 1-Undecen-4-ol

14320-37-1P, Cylopent-3-en-1-one 1545-49-8P 1818-73-7P

14815-14-8P 15222-96-9P 15871-80-3P 16178-87-3P

16215-11-5P 16434-35-4P 16515-55-8P 16717-84-3P

16818-61-4P 1805-02-4P 1855-05-3P 1995-05-3P

19041-66-0P 1975-23-9P 20068-10-4P, (E)-4-Pheyl-3-

butenenitrile 20202-62-4P 20230-16-4P 20337-99-9P

20461-31-8P 21473-05-2P 21488-83-5P, (E)-1-Phenyl-3-

dimehylocta-2,6-diene 21677-96-3P 21886-69-1P 22564-22-1P

22855-55-3P, Mehyl 3-methyl-2-butenoate 26450-24-8P

26561-31-9P 28828-49-8P

27828-12-7P 28973-98-0P 28983-37-8P 29330-79-5P

31666-74-7P 31666-77-0P 31985-02-1P 32064-72-5P,



105-99-0, 1,3-Butadiene, reactions 107-06-2, 1,2-Dichloroethane, reactions 107-83-5, 2-Methylpentane 108-10-1, 4-Methyl-2-pentanone 108-38-5, m-Xylene, reactions 108-65-6, 1-Methoxy-2-propylacetate 108-88-3, Toluene, reactions 109-66-0, Pentane, reactions 110-54-3, Hexane, reactions 111-76-7, 2-Butoxyethanol 115-07-1, Propylene, reactions 115-10-6, Dimethylhept-123-86-4, Butyl acetate 141-18-6, Ethyl acetate, reactions 142-02-5, n-Heptane, reactions 590-18-1, cis-2-Pentene 646-94-8, trans-2-Pentene 7197-62-8, Butyl glycolate 7446-09-5, Sulfur dioxide, reactions 7654-41-7, Ammonia, reactions 11104-93-1, Nitrogen oxide, reactions

RU: OCU (Occurrence, unclassified); POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)

(ground-level ozone formation in relation to speciated volatile organic compound emission inventory in UK)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 30 OF 67 HCAPLUS DOCUMENT NUMBER: 2001-808833 ACCESSION NUMBER: 13615517

TITLE: Characterization of the reactivities of volatile organic compounds using a master chemical mechanism

AUTHOR(S): Derwent, Richard G.; Jenkin, Michael E.; Saunders, Sandra M.; Pilling, Michael J.

CORPORATE SOURCE: Climate Research Division, Meteorological Office, Bracknell, UK

SOURCE: Journal of the Air & Waste Management Association (2001), 51(5), 699-707

CODEN: JAWMFC; ISSN: 1096-2247

PUBLISHER: Air & Waste Management Association

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 07 Nov 2001

AB A comprehensive description of the O<sub>3</sub>-forming potential of 101 organic compds. was developed under North American urban averaged conditions using a detailed master chemical mechanism and a simple air parcel trajectory model. This chemical mechanism describes reactions of 3601 chemical species occurring in >10,500 chemical reactions. An index value, calculated for each organic compound, describes the increment in O<sub>3</sub> concentration observed downwind from an urban area following emission of a fixed increment in the mass emission of each organic compound. These indexes, termed photochm. O<sub>3</sub> creation potentials (POCP), were expressed on a scale relative to ethylene (ethylene) = 100; a reactivity scale was generated for alkanes, alkenes, and oxygenated and halogenated organic compds. A high degree of correlation ( $R^2 = 0.9$ ) was observed between these POCP values and the most widely accepted urban reactivity scale. While reactivity of most of the 86 organic compds. compared fell within a consistent range, significant discrepancies were noted for only 5 compds. Single- or multi-day conditions appeared important in establishing quant. reactivity scales for less reactive organic compds.

IT 78-79-5, Isoprene, reactions 79-20-9, Methyl acetate 107-31-3, Methyl formate 108-21-4, Isopropylacetate 108-60-4, n-Propylacetate 123-86-4, n-Butylacetate 141-78-6, Ethyl acetate, reactions 540-88-5, tert-Butylacetate

RU: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)

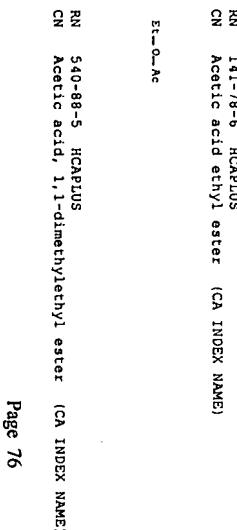
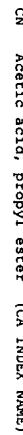
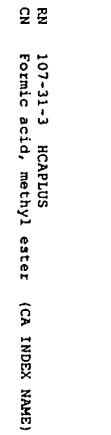
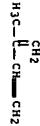
(Reactant or reagent)

(master chemical mechanism model to characterize atmospheric reactivity of volatile organic compds. and their ozone formation potential under North American urban average conditions)

RN 78-79-5 HCPLUS CN 1,3-Butadiene, 2-methyl-

RN 141-78-6 HCPLUS RN 540-88-5 HCPLUS CN Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)

CN Acetic acid, methyl ester (CA INDEX NAME)



CC 59-2 (Air Pollution and Industrial Hygiene)  
 IT Section cross-reference(s): 53  
 50-00-0, Formaldehyde, reactions 57-55-6, Propylene glycol,  
 reactions 60-19-, Diethyl ether, reactions 57-55-6, Propylene glycol,  
 alcohol, reactions 64-18-6, Formic acid, reactions 64-19-7,  
 acetic acid, reactions 67-55-1, Methyl alcohol, reactions 67-66-3,  
 Isopropanol, reactions 67-66-3, Chloroform, reactions 71-23-8,  
 n-Butanol, reactions 71-38-3, n-Butanol, reactions 71-38-3, n-Butanol,  
 Ethane, reactions 74-83-1, Ethylene, reactions 74-83-1, Ethylene, reactions  
 74-83-1, Methyl chloride, reactions 74-98-6, Propane, reactions  
 75-07-0, Acetaldehyde, reactions 75-09-2, Methyne chloride,  
 reactions 75-28-5, Isobutane 75-65-0, tert-Butanol, reactions  
 75-83-2, 2,2-Dimethylbutane 75-85-4, 2-Methyl-2-butanol,  
 reactions 75-97-8, Methyl-tet-butylketone 78-78-4, Isopentane  
 78-79-5, Isoprene, reactions 78-81-1, Isobutanol,  
 reactions 78-94-2, Isobutyraldehyde 78-92-2, sec-Butanol  
 78-93-3, Methylbiketon, reactions 79-01-6, Trichloroethylene, reactions 79-09-4, Propionic acid, reactions  
 79-20-9, Methyl acetate 79-28-8, 2,3-Dimethylbutane  
 80-56-8,  $\alpha$ -Pinene 96-14-0, 3-Methylenepentane 96-22-0,  
 Diethylketone 106-97-8, n-Butane, reactions 106-98-9, But-1-ene, reactions 106-99-0,  
 1,3-Butadiene, reactions 107-21-1, Ethylene glycol, reactions  
 107-31-3, Methyl formate 107-83-5, 2-Methylpentane  
 107-67-9, Methylisobutyketone 107-98-2, 1-Methoxy-2-propanol  
 108-10-1, Methylisobutylketone 107-98-2, 1-Methoxy-2-propanol  
 108-21-4, Isopropylacetate 108-93-0, Cyclohexanol,  
 reactions 108-94-1, Cyclohexone, reactions 108-60-4,  
 n-Propylacetate 109-66-0, n-Pentane, reactions 109-67-1,  
 Pent-1-ene 109-68-4, 2-Methoxyethanol 110-54-3, n-Hexane,  
 reactions 110-62-3, Valeraldehyde 110-80-5, 2-Ethoxymethanol  
 110-82-7, Cyclohexane, reactions 111-65-9, n-Octane, reactions  
 111-76-2, 2-Butoxyethanol 111-84-2, n-Nonane 112-40-3,  
 n-Dodecane 115-10-6, Propene, reactions 115-10-6,  
 Dimethylether 123-38-6, Propionaldehyde, reactions 123-42-2,  
 Diacetylone alcohol 123-51-1, 3-Methyl-1-butanol 123-52-8,  
 Butyraldehyde 123-61-6, n-Butyryacetate 124-18-5,  
 n-Decane 127-18-4, Tetrachloroethyketone  
 2-Methyl-1-butanol 141-76-6, Ethyl acetate, reactions 137-32-6,  
 142-82-5, n-Heptane, reactions 156-59-2, cis-Dichloroethylene  
 156-60-5, 46-02-1, Neopentane 513-35-9, 2-Methylbut-2-ene  
 563-08-8, tert-Butylacetate 563-45-1, 3-Methylbut-1-ene  
 563-46-2, 2-Methylbut-1-ene 563-80-4, Methylisopropylketone  
 584-02-1, 3-Pentanol 569-34-4, 3-Methylhexane 589-38-8,  
 Hexan-3-one 590-18-1, cis-But-2-ene 591-76-4, 2-Methylhexane  
 591-82-6, Hexan-2-one 592-41-6, Hept-1-ene, reactions 598-75-4,  
 3-Methyl-2-butanol 624-64-6, trans-But-2-ene 627-20-3,  
 cis-But-2-ene 637-22-3, Ethyl-tet-butyl ether 646-04-8,  
 trans-But-2-ene 1120-21-4, n-Undecane  
 Methyl-tert-butyl-ether 2278-22-0, Peroxacyetyl nitrate  
 4050-45-7, trans-Hex-2-ene 5131-66-8, 1-Butoxy-2-propanol  
 7688-21-3, cis-Hex-2-ene 7691-37-2, Nitric acid, reactions  
 10102-43-9, Nitric oxide, reactions 10102-44-0, Nitrogen  
 dioxide, reactions 11104-93-1, Nitrogen oxide, reactions  
 23167-67-3, Butylene 11104-93-1, Nitrogen oxide, reactions  
 R1: POI (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT  
 (Reactant or reagent)  
 (master chemical mechanism model to characterize atmospheric reactivity  
 of volatile organic compds. and their ozone formation potential

L74 ANSWER 31 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
 DOCUMENT NUMBER: 2001:43106 HCAPLUS Full-text  
 TITLE: Prediction of flammability of gases by using  
 F-number analysis  
 AUTHOR(S): Kondo, S.; Urano, Y.; Tokuhashi, K.;  
 Takahashi, A.; Tanaka, K.  
 CORPORATE SOURCE: Research Institute of Innovative Technology  
 for the Earth, National Institute of Materials  
 and Chemical Research, Tsukuba, Ibaraki,  
 305-0046, Japan  
 JOURNAL: Journal of Hazardous Materials (2001  
 ), 82(2), 113-128  
 CODEN: JHMAD9; ISSN: 0304-3894  
 ELSEVIER SCIENCE B.V.  
 Journal

SOURCE: ED Entered STN: 28 Feb 2001  
 AB A method of predicting flammability limits uses a flammability index called F-number  
 For this purpose, an empirical expression of F-number was derived to account for the  
 flammability characteristics of various organic substances. The anal. was done by  
 fitting to the observed values of F-number for a wide variety of organic gases and  
 vapors. F-number is an excellent tool to analyze the flammability characteristics of  
 various substances. Upper and lower flammability limits can be derived from F-number  
 together with the stoichiometric concentration corrected for the effect of selective  
 diffusion.

IT 78-79-5, Isoprene, reactions 79-20-9,  
 Methylacetate 80-62-6, Methylmethacrylate  
 96-33-3, Methyl acrylate 96-34-4, Methyl  
 chloroacetate 105-73-3, Ethylpropionate 107-31-3  
 , Methyl formate 108-05-4, Vinyl acetate, reactions  
 108-21-4, Iso propylacetate 109-60-4,  
 Propylacetate 109-94-4, Ethyl Formate 110-19-0  
 , Isobutyl acetate 110-49-6, Methyl cellosolve acetate  
 111-55-7, Glycol diacetate 113-86-4, Butyl  
 acetate 123-92-2, Isopropyl acetate 140-88-5,  
 Ethyl acrylate 141-32-2, Butyrylacetate 141-78-6  
 , Ethyl acetate, reactions 111-07-9, Ethyl acetoacetate  
 554-12-1, Methylpropionate 552-84-7, Amil acetate  
 Butiformate 628-63-7, Amil acetate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 RN (prediction of flammability of gases by using F-number anal.)

RN 78-79-5 HCAPLUS  
 1,3-Butadiene, 2-methyl- (CA INDEX NAME)  
 H<sub>3</sub>C— $\text{C}=\text{C}$ —CH<sub>2</sub>  
 H<sub>3</sub>C—O— $\text{C}$ —CH<sub>3</sub>

## SN 10/564307 Page 79 of 139 STIC STN SEARCH 5/17/2007

## SN 10/564307 Page 80 of 139 STIC STN SEARCH 5/17/2007

 $\text{I-Pr-O-Ac}$ 

RN 80-62-6 HCAPLUS  
CN 2-Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)

$$\text{H}_2\text{C}=\text{C}(\text{Me})\text{CO}-\text{CH}_2-\text{OAc}$$
 $\text{n-Pr-O-Ac}$ 

RN 96-33-3 HCAPLUS  
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)

$$\text{MeO}-\text{CH}=\text{C}(\text{H}_2)\text{CO}-\text{CH}_2-\text{OAc}$$
 $\text{H}_3\text{C}-\text{CH}_2-\text{O}-\text{CH}_2-\text{OAc}$ 

RN 109-60-4 HCAPLUS  
CN Acetic acid, propyl ester (CA INDEX NAME)

 $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{OAc}$ 

RN 109-94-4 HCAPLUS  
CN Formic acid, ethyl ester (CA INDEX NAME)

 $\text{H}_3\text{C}-\text{CH}_2-\text{O}-\text{CH}_2-\text{OAc}$ 

RN 110-19-0 HCAPLUS  
CN Acetic acid, 2-methylpropyl ester (CA INDEX NAME)

 $\text{i-Bu-O-Ac}$ 

RN 110-49-6 HCAPLUS  
CN Ethanol, 2-methoxy-, 1-acetate (CA INDEX NAME)

 $\text{AcO}-\text{CH}_2-\text{CH}_2-\text{OAc}$ 

RN 111-55-7 HCAPLUS  
CN 1,2-Ethanediol, 1,2-diacetate (CA INDEX NAME)

 $\text{AcO}-\text{CH}_2-\text{CH}_2-\text{OAc}$ 

RN 123-86-4 HCAPLUS  
CN Acetic acid, butyl ester (CA INDEX NAME)

 $\text{n-Bu-O-Ac}$ 

RN 123-92-2 HCAPLUS  
CN 1-Butanol, 3-methyl-, 1-acetate (CA INDEX NAME)

 $\text{AcO}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{OAc}$ 

RN 96-34-4 HCAPLUS  
CN Acetic acid, 2-chloro-, methyl ester (CA INDEX NAME)

$$\text{MeO}-\overset{\overset{\text{O}}{\parallel}}{\underset{\underset{\text{Cl}}{\parallel}}{\text{C}}}-\text{CH}_2-\text{OAc}$$
 $\text{AcO}-\text{CH}_2-\text{O}-\text{CH}_3$ 

RN 105-37-3 HCAPLUS  
CN Propanoic acid, ethyl ester (CA INDEX NAME)

$$\text{EtO}-\overset{\overset{\text{O}}{\parallel}}{\underset{\underset{\text{Et}}{\parallel}}{\text{C}}}-\text{CH}_2-\text{OAc}$$
 $\text{AcO}-\text{CH}_2-\text{O}-\text{CH}_3$  $\text{AcO}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{OAc}$ 

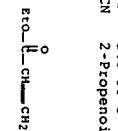
RN 108-05-4 HCAPLUS  
CN Acetic acid ethenyl ester (CA INDEX NAME)

$$\text{AcO}-\text{CH}=\text{CH}_2-\text{OAc}$$
 $\text{AcO}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{OAc}$ 

RN 108-21-4 HCAPLUS  
CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)

$$\text{AcO}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{OAc}$$

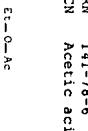
RN 140-88-5 HCAPLUS  
2-Propenoic acid, ethyl ester (CA INDEX NAME)



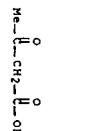
RN 141-32-2 HCAPLUS  
2-Propenoic acid, butyl ester (CA INDEX NAME)



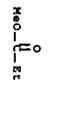
RN 141-78-6 HCAPLUS  
Acetic acid ethyl ester (CA INDEX NAME)



RN 141-97-9 HCAPLUS  
Butanoic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



RN 554-12-1 HCAPLUS  
Propanoic acid, methyl ester (CA INDEX NAME)



CC 59-5 (Air Pollution and Industrial Hygiene)  
IT 57-55-6, Propylene glycol, reactions 60-29-7, Ethylether,  
reactions 62-53-3, Aniline, reactions 64-17-5, Ethyl alcohol,  
reactions 64-18-7, Acetic acid, reactions 67-56-1, Methyl  
alcohol, reactions 67-63-0, Iso propyl alcohol, reactions  
67-64-1, Acetone, reactions 71-23-8, Propyl alcohol, reactions  
71-36-3, Butyl alcohol, reactions 71-41-0, Amyl alcohol,  
reactions 71-43-2, Benzene, reactions 71-55-6,  
1,1,-Trichloroethane 74-62-8, Methane, reactions 74-83-9,  
Methyl bromide, reactions 74-84-0, Ethane, reactions 74-85-1,  
Ethylene, reactions 74-86-2, Acetylene, reactions 74-87-3,  
Methyl chloride, reactions 74-88-5, Methylamine, reactions  
74-96-4, Ethyl bromide 74-98-6, Propane, reactions 75-00-3,  
Ethyl chloride 75-01-4, Vinylchloride, Reactions 75-02-5,  
Vinylfluoride 75-04-7, Ethylamine, reactions 75-05-8,  
Acetonitrile, reactions 75-07-0, Acetaldehyde, reactions  
75-09-2, Methylane, chloroform, reactions 75-10-5 75-19-4  
Cyclopropane 75-21-8, Ethylene oxide, reactions 75-28-5, Iso  
butane 75-29-6, Iso propyl chloride 76-33-4, Vinylidene  
chloride, reactions 76-83-1, Iso butyl alcohol, reactions  
76-84-2 78-87-3, Propylene dichloride 78-88-6,  
2,3-Dichloropropene 78-92-2, 2-Butanol 78-94-4, Methyl vinyl  
ketone, reactions 79-01-6, Trichloroethylene, reactions  
79-03-4, Propionic acid, reactions 79-10-7, Acrylic acid,  
reactions 79-20-3, Methylacetate 79-29-8,  
2,3-Dimethylbutane 79-31-2, Iso butyric acid 79-46-9,  
2-Nitropropane 80-62-6, Methylmethacrylate 85-44-9,  
Phthalic anhydride 91-20-3, Naphthalene, reactions  
92-52-4, Biphenyl, reactions 95-47-6,  $\alpha$ -kynen, reactions 95-50-1,  
 $\alpha$ -Dichlorobenzene 96-14-0, 3-Methylpentone 96-33-3,  
Methyl acrylate 96-34-4, Methyl chloroacetate 96-37-7,  
Methylcyclopentane 97-17-3, Isobutyric anhydride 97-96-1  
97-99-4, Tetrahydrofurfuryl alcohol 98-00-0, Furfuryl alcohol  
98-01-1, Furan, reactions 98-06-6, Tert Butylbenzene  
98-82-8, Cumene 100-41-4, Ethylbenzene, reactions 100-62-5,  
Styrene, reactions 103-09-3, 2-Ethylhexylacetate 103-65-1,  
Propiophenone 104-51-8, Butylbenzene 104-76-7, 2-Ethylhexanol  
105-05-5,  $\rho$ -Diethylbenzene 105-30-6 105-37-3,  
Ethylpropionate 105-46-4, Sec Butyl Acetate 105-57-7, Acetal  
106-31-0, Butyric anhydride 106-42-3,  $\rho$ -Xylene, reactions  
106-88-7, 1,2-Butylene oxide 106-89-8, Epichlorohydrin,  
reactions 106-95-5, Allyl bromide, reactions 106-97-8, Butane,  
reactions 106-98-9, 1-Butene, reactions 106-99-0,  
1,3-Butadiene, reactions 107-02-8, Acrolein, reactions  
107-05-1, Allyl chloride 107-06-2, Ethylene chloride, reactions  
107-07-3, 2-Chloroethanol, reactions 107-10-8, Propylamine,  
reactions 107-11-9, Allylamine 107-13-1, Acrylonitrile,  
reactions 107-15-3, Ethylenediamine, reactions 107-18-6, Allyl  
alcohol, reactions 107-31-3, Methyl formate 107-83-5,  
Isohexane 107-77-9, Methylirocyanopropene  
reactions 108-05-4, Vinyl acetate, reactions 108-10-1,  
Methyl isobutyl ketone 108-11-2, Methyl isobutylcarbinol  
108-18-9, Di-isopropylamine 108-20-3, Isopropyl ether  
108-21-4, Iso propylacetate 108-24-7, Acetic anhydride  
108-31-6, Maleic anhydride, reactions 108-38-3, reactions

RN 628-63-7 HCAPLUS  
Acetic acid, pentyl ester (CA INDEX NAME)

SN 10/564307 Page 83 of 139 STIC STN SEARCH 5/17/2007

108-33-8, Di-isobutylketone 108-84-9 108-87-2,  
Methylcyclohexane 108-88-3, Toluol, Reactions 108-90-7,  
Chlorobenzene, Reactions 108-94-1, Cyclohexanone, Reactions  
109-60-4, Propylacetate 109-65-9, Butyl bromide  
109-66-0, Pentane, Reactions 109-67-1, 1-Pentene 109-69-3,  
Butyl chloride 109-73-9, Butylamine, Reactions 109-87-5,  
Methylal 109-89-7, Diethylamine, Reactions 109-92-2, Vinyl  
ethyl ether 109-93-3, Divinyl ether 109-94-4, Ethyl  
formate 109-99-9, Tetrahydrofuran, Reactions 110-00-9, Furan  
110-12-3, Methylisomyrketone 110-19-0, Isobutyl acetate  
110-43-0, Methylamyl ketone 110-45-6, Methyl cellosolve  
acetate 110-54-3, Hexane, Reactions 110-88-3, Trioxane, Reactions  
110-92-7, Cyclohexane, Reactions 110-98-3, Diethylbenzene triamine  
110-91-8, Morholine, Reactions 111-40-0, Diethylene triamine  
111-43-3, n-Propyl ether 111-55-7, Glycol dicetate  
111-85-9, Octane, Reactions 111-84-2, Nonane 112-27-6,  
Triethylene glycol 115-07-1, Propylene, Reactions 115-06-6,  
Methylmethane 115-11-7, 2-Methylpropane, Reactions 116-14-3,  
Tetraisopropylmethane, Reactions 123-05-7, 2-Ethylhexanol  
123-20-6, Vinylbutyrate 123-42-2, Diacetone alcohol 123-51-3,  
Isomethyl alcohol 123-62-6, Propionic anhydride 123-72-8, Butyl  
aldehyde 123-86-4, Butyl acetate 123-91-1, P-Dioxane,  
reactions 123-92-2, Isomethyl acetate 124-18-5, Decane  
124-40-3, Dimethylamine, Reactions 126-98-7, Methylacrylonitrile  
126-99-8, 3-Chloro-3,3-budadiene 135-98-8, Sec Butylbenzene  
140-88-5, Ethyl acrylate 141-32-2, Butylacrylate  
141-78-6, Ethyl acetocetate, Reactions 141-79-7, Methyl  
oxide 141-97-9, Ethyl acetoacetate 142-82-5, Heptane,  
reactions 142-96-1, Dimethylamine, Reactions 149-57-5,  
151-56-4, Ethylenimine, Reactions 219-1-64-5, Cyclohexanone  
430-65-0, 1,1,2-trichloroethane 463-82-1, 2,2-Dimethylpropane  
513-16-0, Iso butyl chloride 538-93-2, IsoButylbenzene  
540-59-5, Propyl chloride 540-59-0, 1,2-Dichloroethane  
549-67-0, Methyl ethyl ether 549-55-2, 1,50 butylformate  
542-75-6, 1,3-Dichloropropane 554-12-1, Methylpropionate  
563-45-1, 3-Methyl-1-butene 563-47-3, Methylallyl chloride  
564-02-3, 2,2,3-Trimethylpentane 565-59-3, 2,3-Dimethylpentane  
584-02-1, 3-Pentanol 589-38-8, 3-Hexanone 590-18-1,  
cis-2-Butene 590-31-6, 1-Chloropropane 591-97-9, 592-45-0,  
1,4-Hexadiene 592-84-7, Butylformate 593-53-3, Methyl  
fluoride 593-60-2, Vinylbromide 593-70-4, Chlorofluoromethane  
594-36-5, Tert Amyl chloride 624-64-5, trans-2-Butene  
627-21-0, 3-Buten-1-ol 628-37-0, Ethylpropylether  
628-63-7, Amyl acetate 821-55-6, Methylheptylketone  
629-2-Butene 590-31-6, 1-Chloropropane 591-97-9, 592-45-0,  
1,4-Hexadiene 592-84-7, Butylformate 593-53-3, Methyl  
fluoride 593-60-2, Vinylbromide 593-70-4, Chlorofluoromethane  
1067-20-5, 3,3-Diethylpentane 1121-74-0, Divinylbenzene,  
reactions 131-43-7, Diethylcyclohexane 1640-89-7,  
Ethylcyclopentane 1653-19-6, 2,3-Dichlorobutadiene-1,3  
1678-91-7, Ethylcyclohexane 1711-00-6, 1,1'-Bifluoro-1,1'-  
dichloroethane 326-23-7, 2,3-Butylene oxide 4170-30-3,  
Crotonealdehyde 4401-11-0, 2-Chloro-2-butene 4784-77-4, Crotyl  
bromide 4806-61-5, 1,1-Dihydrocyclobutene 6117-91-5, Crotonyl  
alcohol 7156-79-2, 2,2,3,3-Tetramethylpentane 12002-08-1,  
Trichlorobenzene 25013-15-4, Vinyltoluene 25167-70-8,  
2,2,4-Trimethylpentane 25551-13-7, Trimethylbenzene  
25567-67-3, Dinitrochlorobenzene 26519-91-5,  
Methylcyclopentadiene 26635-62-2, Sec Amyl alcohol 31394-54-4,  
Isobutane 62310-91-7, Propional 80466-41-8, 2,4-Hexadienal  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prediction of flammability of gases by using F-number anal.)  
REFERENCE COUNT: 7  
THERE ARE 7 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

174 ANSWER 32 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1999-13566 HCAPLUS Full-text  
DOCUMENT NUMBER: 1304143109

SN 10/564307 Page 84 of 139 STIC STN SEARCH 5/17/2007

TITLE:

PoCP for individual VOC under European conditions

Allendeet, Johanna; Pleijel, Karin  
Goteborg, Sweden

AUTHOR(S):

CORPORATE SOURCE:

IWL Report (1998), B 1105, 1-47

SOURCE:

CODEN: IWLBD0; ISSN: 0347-8896

DOCUMENT TYPE:

Report

LANGUAGE:

English

ED Entered STN: 11 Jan 1999

AB AB

03 production from volatile organic compds. (VOC) in the atmospheric is discussed, focusing on a general way to present photochem. 03 creation potential (PoCP) values for different VOC under European conditions and to calculate such values for a large number of VOC. Topics discussed include: environmental impact of VOC in atmosphere; tropospheric 03; the photo-oxidative environment; NOx and VOC precursors of tropospheric 03; atmospheric chemical of VOC; ranking VOC according to their ability to produce 03; methods for critical anal. of PoCP concept; results from critical anal. of the PoCP concept; selecting model set-up to calculate PoCP; PoCP under European conditions; and conclusions.

IT 78-79-5, Isoprene, Reactions 79-20-9,

Methylacetate 123-86-4, n-Buylacetate 141-78-6

RL: POI (Pollutant); RCM (Reactant); OCCU (Occurrence); RACT

(Reactant or reagent)

(modeling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

RN 78-79-5 HCAPLUS

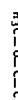
CN 1,3-Butadiene, 2-methyl-

(CA INDEX NAME)



RN 79-20-9 HCAPLUS  
CN Acetic acid, methyl ester (CA INDEX NAME)

RN 123-86-4 HCAPLUS  
CN Acetic acid, butyl ester (CA INDEX NAME)



E1-O-Ac

CC 59-2 (Air Pollution and Industrial Hygiene)



RN 115-95-7 HCAPLUS  
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

CC 30-10 (Terpenes and Terpenoids)  
IT 123-35-3B, Myrcene, hydrochlorination products  
NAME)

IT 471-10-3 Linalyl chloride  
20536-36-1, Neryl chloride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

IT 105-87-3P, Geranyl acetate  
acetate 141-12-8P, Neryl acetate  
(synthetic preparation); PREP (Preparation)

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
(cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

L74 ANSWER 34 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1997-62046 HCAPLUS Full-text  
DOCUMENT NUMBER: 126-157642

TITLE: Research and development in synthesis of series fine chemicals from rosin and turpentine. IV. Synthesis of neryl and geranyl acetates

AUTHOR(S): Li, Qiahe; Yin, Dulin; Li, Haorui; Lin, Lihen; Ma, Runwei  
CORPORATE SOURCE: Institute of Fine Catalysis and Synthesis, Hunan Teacher's University, Changsha, 410081, People Rep. China  
SOURCE: Hunan Shifan Daxue Ziran Kexue Xuebao (1996), 19(3), 34-37  
CODEN: HSDEBL; ISSN: 1000-2537

PUBLISHER: Hunan Shifan Daxue Qikansha  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese  
ED Entered STN: 29 Jan 1997

AB Neryl and geranyl acetates were synthesized from  $\beta$ -pinene in turpentine oil by a 3-step process consisting of catalytic isomerization, hydrochlorination, and esterification. The effect of the esterification conditions on the yield of the title compds. was studied. In the presence of 2% Et<sub>3</sub>N (the catalyst) myrcene hydrochlorination crude products reacted with equimolar anhydrous NaOAc at 85-90° for 5 h, the total yield of the 2 title esters reached 66.6% based on  $\beta$ -pinene, in which ester products the selectivity of neryl acetate was 40-45% whereas that of geranyl acetate was 55-60%.

IT 123-35-3B, Myrcene, hydrochlorination products  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 123-35-3 HCAPLUS

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

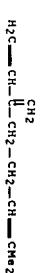
IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\beta$ -Pinene conversion to neryl acetate and geranyl acetate)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

PUBLISHER: Pharmaceutical Society of Japan  
Page 88

RN 123-35-3 HCAPLUS  
1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



**SN 10/564307 Page 92 of 139 STIC STN SEARCH 5/17/2007**

exo tandem cyclization to *cis*-3-oxa-4-silacyclo[4.3.0]nonanes I (R<sup>2</sup> = H, CH<sub>2</sub>COPMe), and 3-oxa-2-silatetradeca-5,9,13-trien-1-yl radicals sequential 6-endo-6-endo-5-exo triple cyclization to *trans*-*trans*-*trans*-12-oxa-11-silatricyclo[7.4.0.0.0.6]tridecanes (II). Vitamin B12

IT 68-19-9, Vitamin B12  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(catalyst for reductive radical cyclization of terpenoid bromocetals or bromomethylsilyl ether)

RN 68-19-9 HCAPLUS  
CN Vitamin B12 (CA INDEX NAME)

## CC 30-1 ("Terpenes and Terpenoids")

Section cross-reference(s): 5, 22  
IT 76-49-3, Bornyl acetate 79-92-5, Camphene 80-56-8,  
a-Pinene 89-78-1, Menthol 89-80-5, Menthone 89-82-7  
99-48-9 99-86-5,  $\alpha$ -Terpinene 99-87-6,  $\beta$ -Cymene  
105-87-3, Geranyl acetate 106-24-1, Geraniol 106-25-2,  
Nerol 115-93-7, Linyl acetate 123-35-3,  
Myrcene 127-91-3,  $\beta$ -Pinene 138-86-3, Limonene 464-18-2,  
(1S)-(-)-Camphor 470-82-6, 1,8-Cineole 501-52-0, Hydrocinnamic acid 562-24-3, 4-Terninal 1135-24-6, Ferulic acid 116-01-6  
2009-00-9, (+)-Sabinene 2244-16-8, (S)-(+)-Carvone 7764-50-3  
1848-59-6, (1R)-Myrtenol 139894-97-4, (1R)-(-)-Myrtenol 2267-21-1, 3271-61-2, Epivodone 113412-11-6, Calaminthone 131549-80-9, Desacetylcalaminthone

RL: RCT (Reactant); RACT (Reactant or reagent)  
(water solubility of, determination of, via gas chromatogr.)

L74 ANSWER 37 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1991:164539 HCAPLUS Full-text  
DOCUMENT NUMBER: 114:164539

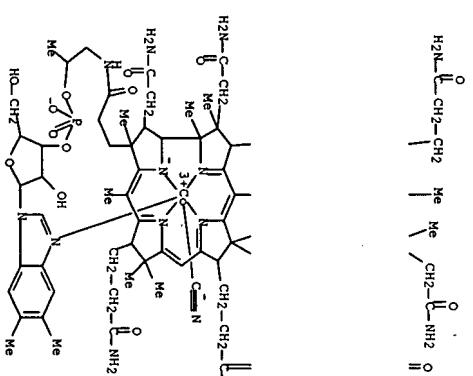
TITLE: Reductive radical cyclizations of bromo acetals and (bromomethyl)silyl ethers of terpenoid acetals

AUTHOR(S): Lee, Edward R.; Lakomy, Ivo; Bigler, Peter;  
Scheffold, Rolf  
Inst. org. Chem., Univ. Bern, Bern, CH-3012,  
Switz.

CORPORATE SOURCE: Helvetica Chimica Acta (1991),  
74(1), 146-152

SOURCE: CODEN: HCACV; ISSN: 0018-019X  
Journal

DOCUMENT TYPE: OTHER SOURCE(S): English  
LANGUAGE: CAreact 114:164539  
ED Entered STN: 03 May 1991  
GI



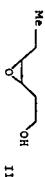
PAGE 2-A

**AB** The tin hydride promoted and the reductive vitamin B12 catalyzed radical cyclization of mixed 2-bromocetals/alkyldiene acetals and of (2-bromomethyl)dimeethylsilyl ethers of allylic terpenoid alcs. was investigated: 3-oxadeca-5,9-dien-1-yl radicals undergo 5-exo cyclization to oxolanes, 3-oxa-2-siladeca-5,9-dien-1-yl radicals sequential 6-endo-5-

IT 105-45-3, Methyl acetoacetate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(diamon alkyl)ation of, with siloxygeranyl bromide)

RN 105-45-3 HCAPLUS  
CN Butanoic acid, 3-oxo-, methyl ester (CA INDEX NAME)

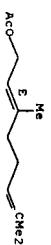
DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 123:339558  
 ED Entered STN: 17 Aug 1985  
 GI



AB A reagent combination system, tetracyanoethylene (I) -10% H<sub>2</sub>O<sub>2</sub>, epoxidized olefins efficiently in MeCN at room temperature in a stereospecific manner with retention of the configuration of the double bond. H<sub>2</sub>O<sub>2</sub> 30% was added to I and cis-3-hexen-1-ol in MeCN at room temperature for 12 h to give cis-II. Was acetate, 105-87-3 123-35-3 540-88-5, tert-Butyl acetoacetate (Reactant); RACT (Reactant or reagent) (tetracyanoethylene-hydrogen peroxide, a mild epoxidin. system of olefins)

RN 105-87-3 HCAPLUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS  
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 540-88-5 HCAPLUS  
 CN Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)

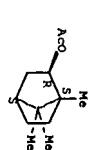


CC 27-2 (Heterocyclic Compounds (One Hetero Atom))  
 IT 105-87-3 106-23-0 106-24-1 106-98-5, Benzenethiol, reactions 110-93-0 123-35-3 540-88-5, tert-Butyl acetate 870-61-3 1-Bromo-3-methyl-2-butene, 928-96-1, cis-3-Hexen-1-ol 3695-38-3 4222-94-6 42602-37-9 5113-72-5 5218-73-5 76811-78-8 88191-39-3 RL: RCT (Reactant); RACT (Reactant or reagent) (tetracyanoethylene-hydrogen peroxide, a mild epoxidin. system of olefins)

L74 ANSWER 36 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1994-8750 HCAPLUS Full-text  
 DOCUMENT NUMBER: 120-8750  
 TITLE: Just how insoluble are monoterpenes?  
 AUTHOR(S): Weidenmaier, Jeffrey D.; Macias, Francisco A.; Fischer, Nikolaus H.; Williamson, G. Bruce  
 CORPORATE SOURCE: Dep. Chem., Louisiana State Univ., Baton Rouge, LA 70803 USA  
 Journal of Chemical Ecology (1993), 19(8), 1799-807  
 CODEN: JCEDD8; ISSN: 0098-0331

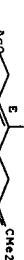
SOURCE: English  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 08 Jan 1994  
 AB Prior generalizations about the eccl. roles of monoterpenes may be misleading if based on the presumed insolv. of monoterpenes in water. The authors determined the aqueous solubility of 31 biol. active monoterpenes by gas chromatog. While hydrocarbons were of low solubility (<35 ppm), oxygenated monoterpenes exhibited solubilities one or two orders of magnitude higher, with ranges of 155-6590 ppm for ketones and of 103-1360 ppm for alcs. Many monoterpenes are phytotoxic in concns. under 100 ppm, well below the saturated aqueous concns. of oxygenated monoterpenes. Therefore, even dilute, unsat. soins. or monoterpenes, occurring naturally in plant tissues and soil solns., may act as potent biol. inhibitors.  
 IT 76-49-3, Bornyl acetate 305-9-3, Geranyl acetate 115-95-7, Linalyl acetate 123-35-3,  
 Myrcene  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 RN 76-49-3 HCAPLUS  
 CN Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, 2-acetate, (IR, 2S, 4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 105-87-3 HCAPLUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 115-95-7 HCAPLUS  
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)

H<sub>2</sub>C—CH—<sup>CH<sub>2</sub></sup>—CH<sub>2</sub>—CH—CMe<sub>2</sub>  
 Me



SN 10/564307 Page 96 of 139 STIC STN SEARCH 5/17/2007  
(Preparation and saponification of)

LANGUAGE: Chinese

ED Entered STN: 12 Jan 1991

The synthetic route of geraniol and nerol was studied. Myrcene which was obtained from  $\beta$ -pinene in gum turpentine by heat isomerization was used as raw material. In the presence of catalyst, myrcene was treated by addition of HCl to form an adduct mixture consisting mainly of geranyl chloride and neryl chloride with small amounts of other chlorides such as linalyl chloride and turpental chloride present. These then converted sep. to their resp. acetate esters by treatment with sodium acetate in the presence of a catalyst. The major products are geranyl acetate and neryl acetate. The yield of the acetates was 50-60%, and the ratio of geranyl acetate to neryl acetate in the mixed esters was about 6:4. Affecting factors as temperature, solvents, catalysts and reaction time were investigated. Saponification of the acetates produced the resp. alcs. Pure geraniol and nerol were separated by rectification on a highly efficient packed column.

IT RL: RCT (Reactant); RACT (Reactant or reagent)

RN 123-35-3 HCPLUS 1,6-Octadiene, 7-methyl-3-methylene-

(CA INDEX NAME)



IT RL: (Chlorination of)

RN 123-35-3 HCPLUS

1,6-Octadiene, 7-methyl-3-methylene-

(CA INDEX NAME)

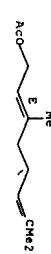
IT RN 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 105-87-3 HCPLUS 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)-

(CA INDEX NAME)

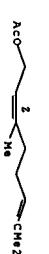
Double bond geometry as shown.



IT RN 141-12-8 HCPLUS 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-

(CA INDEX NAME)

Double bond geometry as shown.



IT RN 141-12-8 HCPLUS 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-

(CA INDEX NAME)

IT RN 123-35-3, Myrcene RL: RCT (Reactant); RACT (Reactant or reagent)

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

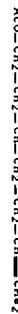
IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

Page 95

Page 96





CC 30-10 (Terpanes and Terpenoids)

IT 105-7-3 115-95-7 123-35-3

RU: RCT (Reactant); RACT (Reactant or reagent)

(allylic chlorination of, by sulfonyl chloride)

L74 ANSWER 42 OF 67 HCPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1189-53484 HCPLUS Full-text

DOCUMENT NUMBER:

TITLE:

Reaction of sulfoxide hydrochlorides and hydrobromides with trisubstituted olefins

Moiseenkov, A. M.; Dragun, V. A.; Lozanova, A.

V. I.; Veselovskii, V. V.

Inst. Org. Khim. im. Zelinskogo, Moscow, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1988), (8), 1797-803

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE:

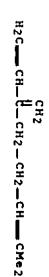
Language: Russian

OTHER SOURCE(S): CASREACT 111:134484

ED Entered SIN: 14 Oct 1988  
Chlorination of Me2C:CHCH2CH2C(:X)Me (X = H, OAc, H, CH2CH2OAc; CHCH2OAc) by R12SO-HCl [R1 = Me, Ph, R12 = (CH2)4] in MeNO2 or CH2Cl2 containing CaCl2 or LiClO4 or by Cl2-CCl4 at -50° or by HCl-AcOH at 0° gave mixts. containing CH2:CHCH2CH2C(:X)Me whose yields and ratios depended on the process. Addnl. obtained were some bromo derivs.

IT 123-35-3 RCT (Reactant); RACT (Reactant or reagent)

RN 123-35-3 HCPLUS  
1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

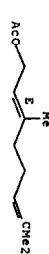


IT 105-87-3 150-84-5

RU: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination and bromination of, by sulfoxide hydrochlorides and hydrobromides)

RN 105-87-3 HCPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpanes and Terpenoids)

IT 123-35-3 Section cross-reference(s): 23

RU: RCT (Reactant); RACT (Reactant or reagent)

(bromination of)

IT 105-87-3 150-84-5 19162-00-6

RU: RCT (Reactant); RACT (Reactant or reagent)

(chlorination and bromination of, by sulfoxide hydrochlorides and hydrobromides)

L74 ANSWER 43 OF 67 HCPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1988-93347 HCPLUS Full-text

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1987), (12), 2787-90

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

Language: Russian

OTHER SOURCE(S): CASREACT 109:93347

ED Entered SIN: 17 Sep 1988  
Treating RCH:CHMe2 [R = CH2CH2C(:CH2)CH:CH2, trans- and cis-CH2CH2CHMe:CHCH2OAc, CH2CH2CMe:CHCH2OAc] with PISOCl in Me2CHNO2 containing ZnCl2 gave 50-65% of P(OMe)3-MeOH to give 85-90% R-CH:CH(OH). Grignard reaction of I (R = CH2CH2C(:CH2)CH:CH2) in the presence of Me2S:CHCH2Cl in the presence of CuI-THF gave 34% of a 4:1 E/Z mixture of Me2C:CHCH2CH2Me:CHCH2CH2C(:CH2)CH:CH2.

IT 105-87-3 123-35-3 141-12-8

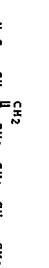
RU: RCT (Reactant); RACT (Reactant or reagent)

RN 105-87-3 HCPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCPLUS  
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



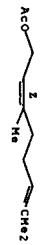
RN 150-84-5 HCPLUS  
6-Octen-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX  
NAME)

Double bond geometry as shown.



Double bond geometry as shown.



RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX  
NAME)

Double bond geometry as shown.

CC 30-15 (Terpenes and Terpenoids)  
IT 195-57-3 133-35-3 141-12-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(regioselective ene reaction of, with benzenesulfonyl chloride)

L74 ANSWER 44 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN

DOCUMENT NUMBER: 1988-510661 HCAPLUS Full-text

DOCUMENT NUMBER: 109-110661  
TITLE: Regiospecific ene reaction of benzenesulfonyl chloride with linear isoprenoids

Moisenkov, A. M.; Dragun, V. A.; Koptenkova,

V. A.; Veselovskii, V. V.

N. D. Zelinskii Inst. Org. Chem., Moscow, USSR

SOURCE: Synthesis 1987, (9), 84-15

CODEN: SYNBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109-110661

ED Entered STN: 01 Oct 1988

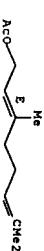
AB Entered STN: 01 Oct 1988  
The Lewis acid (e.g., ZnCl<sub>2</sub>) catalyzed ene reaction of PhSOCl with myrcene, geranyl and neretyl acetates, as well as Et (E,E)-farnesate proceeds smoothly and chemoselectively by exclusive attack at the terminal tri-substituted C:C bond to give allylic sulfonates. IT 105-87-3, Geranyl acetate 133-35-3, Myrcene  
141-12-8, Neryl acetate

RU: RCT (Reactant); RACT (Reactant or reagent)

CN 105-87-3 HCAPLUS  
DOCUMENT NUMBER: 109-110661 HCAPLUS Full-text

NAME) (CA INDEX

Double bond geometry as shown.



RN 123-35-3 HCAPLUS  
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

M<sub>2</sub>C=CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH=CH<sub>2</sub>

RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX  
NAME)

A method is described or manufacturing a tertiary, optionally halogenated allylic ester by the reaction of an alkali metal salt of a carboxylic acid with a primary and/or tertiary allylic halide (prepared by hydrohalogenation of an optionally halogenated polycene containing 2 conjugated double bonds and, optionally, 2 more double bonds). The hydrohalogenation catalyst is composed of a Cu(II) salt (e.g., CuI or CuCl), an ammonium salt (e.g., tetrakis(hexamethylbenzyl)ammonium halide or trialkylamine hydrohalide) or a phosphonium salt (e.g., tetrakis(hexamethylbenzyl)phosphonium halide). The starting material is chosen from myrcene,  $\beta$ -farnesene,  $\beta$ -springene, phytatriene and phyttetraene. Thus, in a reactor under Ar were combined 3.0 mL  $\text{CH}_2\text{Cl}_2$ , Et<sub>3</sub>N·HCl 3.33, CuCl 2.4, and myrcene 164.9 g. The reaction mixture was cooled to -5° and 3 mol HCl was added. After the hydrochlorination step, the solution was added to another reactor, under Ar, containing anhydrous NaOHC 145, CuCl 2.4, and Et<sub>3</sub>N·HCl 3.3 g. CuCl 2.4 g was added and the solution was mixed 18 h at 20°. The reaction mixture was cooled and an intensely blue aqueous phase and a clear brown organic phase were obtained. After decanting, the organic phase was washed with 200 mL aqueous 1.0 g/L NaCl solution, 2 times with 200 mL H<sub>2</sub>O and dried with K<sub>2</sub>CO<sub>3</sub>. After filtration and solvent evaporation, an oil 237.1 g was obtained, containing 59% linalyl acetate. The yield from myrcene was 84.5%. The selectivity for linalyl acetate, expressed as the ratio of linalyl acetate to the sum of linalyl acetate, geranyl acetate, and neryl acetate, was 97%.

RU: RCT (Reactant); RACT (Reactant or reagent)  
 (acetoxylation by, of hydrochlorinated polyenes)  
 RN: 127-99-3  
 HEPOLUS  
 Acetic acid, sodium salt (1:1) (CA INDEX NAME)

No. 1

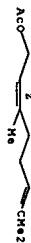
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrohalogenation of, copper halide-quaternary ammonium salt  
 or phosphonium salt-catalyzed)  
 123-35-3 HCAPLUS  
 1,6-octadiene, 7-methyl-3-methylene- (CA INDEX NAME)  
 CN

$$\text{H}_2\text{C}=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CMe}_2$$

IT 58-95-7P

RN: 38-22-5  
CN: 1-Benzoxyan-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-[(4R,8R),  
4,8,12-trimethyltridecyl]-, 6-acetate, (2R)- (CA INDEX NAME)

תְּלִימָדָה בְּבֵית־בְּנֵי־בְּנָה



Page 103

IT 80-26-2P 105-87-3P 115-95-7P

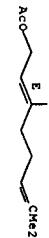
RL: PREP (Preparation)  
RL: PREP (Preparation)  
RL: PREP (Preparation)  
(Manufacturer of, copper chloride-triethylamine hydrochloride-  
141-12-8P

CN  
3-Cyclohexene-1-methanol,  $\alpha$ , $\alpha$ ,4-trimethyl-, 1-acetate  
(CA INDEX NAME)

CC(C)(C)c1ccccc1C(=O)O

RN 105-87-3 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)-  
(CA INDEX NAME)

卷之三



RN 115-95-7  
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME HCAPLUS)

$$\text{H}_2\text{C}=\text{CH}-\overset{\text{ba,c}}{\underset{\text{c}}{\text{C}}} \text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$$

NAME) 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NO  
141-12-0 nuchius CN

despite being geometry as shown

IC ICM CORC067-11  
ICS CORC069-145; CORC069-63  
ICa CORC017-02; CORC021-04  
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)  
Section cross-references(s): 23, 67  
IT Esters, Preparation  
RL: PREP (Preparation)  
(branched,  $\beta$ -unsatd., manufacture of, from hydrohalogenated polyenes, copper halide- and quaternary ammonium or phosphonium salt-catalyzed)

IT 127-09-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acetoxylation by, of hydrohalogenated polyenes)

IT 123-35-3 18194-84-8 70901-63-2 71138-26-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrochlorination by, copper halide-quaternary ammonium salt or phosphonium salt-catalyzed)

IT 58-95-7 p 638-36-8 p  
RL: PREP (Preparation)  
(manufacture of, by hydrogenation)

IT 80-26-2 p 105-87-3 p 115-95-7 p  
RL: PREP (Preparation)  
(manufacture of, copper chloride-triethylamine hydrochloride-catalyzed)

L74 ANSWER 46 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1986:049 HCAPLUS Full-text  
DOCUMENT NUMBER: 104:6049  
TITLE:  
AUTHOR(S): Maeki, Yukio; Sakuma, Kazuhiko; Kaji, Kenji  
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, 502, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(5), 1930-40  
CODEN: CPHBTL; ISSN: 0009-2363  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 104:6049  
ED Entered STN: 11 Jan 1986

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

AB gem-Di-Me olefins, e.g. I (R = O (R1 = PhCH2, Ac, MeOCH2)), OI (R2 = MeO, R22 = benzo, R3 = PhCH2, Me, n = 0) were regioselectively converted to the sulfides II via addition of MeOCS2Cl followed by dehydrochlorination, or chlorination with SOCl2 followed by sulfonylation with MeO2CSH2S. Treatment of II with Me3COK or NaH in DMSO gave esters III by stereoselective desulfurative [2,3]-sigmatropic rearrangement. Dial IV, a component of the pheromonal secretion of the queen butterfly, and quinoid acids V (R2 as above, m = 1,2), metabolites of polyisoprenoid quinones, were prepared by this method.

IT 103-87-3 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination and chlorosulfonylation of, 105-87-3 HCAPLUS 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME))

IT 123-35-3 HCAPLUS  
RN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)  
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

CC=C(C=C)C(C)(C)C=CC=C

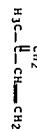
IT 2365-48-2  
RN 2365-48-2 HCAPLUS  
CN Acetic acid, 2-mercaptop-, methyl ester (CA INDEX NAME)

CC(=O)SCC

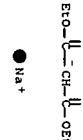
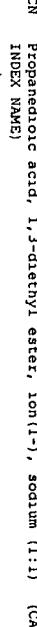
IT 30-40 (Terpenes and Terpenoids) 32247-33-9  
CC 105-77-3 123-35-3 4957-17-9  
RN 52189-73-5 53772-25-1 66958-67-6 70473-30-2 83036-56-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
IT 2365-48-2  
RN (Chlorination and chlorosulfonylation of)  
CN RCT (Reactant); RACT (Reactant or reagent)  
(chlorination and reaction of, with methallyl chlorides)

L74 ANSWER 47 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1986:6027 HCAPLUS Full-text  
DOCUMENT NUMBER: 104:6027  
TITLE:  
AUTHOR(S): Cuvigny, Pierre; Julia, Marc; Roland, C.  
CORPORATE SOURCE: Lab. Chim., Ec. Norm. Super., Paris, 75231/05,  
France  
SOURCE: Journal of Organometallic Chemistry (1985), 285(1-3), 355-113  
CODEN: JORCAT; ISSN: 0022-328X  
DOCUMENT TYPE: Journal  
LANGUAGE: French  
OTHER SOURCE(S): CASREACT 104:6027  
ED Entered STN: 11 Jan 1986  
RL: RCT (Reactant); RACT (Reactant or reagent)  
The influence of the leaving groups, carbanions and ligands on  $\pi$ -allylpalladium has been investigated in the substitution of primary or tertiary terpene derivs., e.g., geranyl acetate, neryl acetate. Conditions have been found under which the substitution takes place essentially at one or the other end of the allylic system. This provides a new and convenient way to obtain compds. with quaternary C's, which has been exemplified by the synthesis of CH2:CHMe2CH2CH3.

IT 78-79-5 reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (addition reaction of, with malonic acid derivs.)  
 RN 78-79-5 HCAPIUS  
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

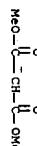


IT 996-82-7 18424-76-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (allylation of, in presence of palladium)  
 RN 996-82-7 HCAPIUS  
 CN Propandioic acid, 1,3-diethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)



● Na+

IT 18424-76-5 HCAPIUS  
 CN Propandioic acid, dimethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)



● Na+

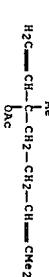
IT 101-02-0 116-17-6  
 RL: CAT (Catalyst use); USES (uses)  
 (catalysts, containing palladium, for substitution of carbanions by  
 allylic derivs.)  
 RN 101-02-0 HCAPIUS  
 CN Phosphorous acid, triphenyl ester (CA INDEX NAME)



IT 116-17-6 HCAPIUS  
 RN Phosphorous acid, tris(1-methylethyl) ester (CA INDEX NAME)

IT 141-12-8 HCAPIUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)  
 Double bond geometry as shown.

IT 115-95-7 HCAPIUS  
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)

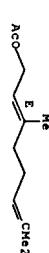


IT 18852-51-2 1922-39-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (addition reaction of, with malonic acid derivs.)  
 IT 996-82-7 18424-76-5 18852-51-2 1922-39-4  
 IT 20330-42-3 24163-38-0 75950-40-7 99372-01-7 99372-24-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 IT 101-02-0 116-17-6 122-52-1 603-35-0, uses

i-Pro-

IT 1191-16-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution by, or carbanions in presence of palladium)  
 RN 105-87-3 HCAPIUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 30-10 (Terpenes and Terpenoids)  
 CC Section cross-reference(s): 22, 29

IT 76-78-5, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)

IT 996-82-7 18424-76-5 18852-51-2 1922-39-4  
 IT 20330-42-3 24163-38-0 75950-40-7 99372-01-7 99372-24-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)

## SN 10/564307 Page 109 of 139 STIC STN SEARCH 5/17/2007

and miscellaneous 1445-83-6 1563-45-2 36238-99-0

RL: CATT (catalyst use); USES (uses)

(catalysts, containing palladium, for substitution of carbanions by

allylic derivs.)

IT 105-87-3 115-95-7 141-12-8 15543-64-3 24509-88-4 68345-17-5

1191-16-8 72863-23-1 72863-21-9 93375-00-6

RN: RCT (Reactant); RACT (Reactant or reagent)

(substitution by, of carbanions in presence of palladium)

L74 ANSWER 48 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985-95834 HCAPLUS Full-text

DOCUMENT NUMBER: 102195834

TITLE: Facile functionalization of the isopropylidene

terminus of acyclic monoolefines by way of

benzenesulfonyl chloride addition

Masaki, Yujiro; Hashimoto, Kinji; Kaji, Kenji

Gifu Coll. Pharm.; Gifu, 502, Japan

Tetrahedron, (1984), 40(18), 3481-90

CODEN: TETRA8; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 22 Mar 1985

AB Addition reaction of  $\text{RCH}_2\text{CH}(\text{OMe})^2$  [R = H, PhCH<sub>2</sub>O, CH<sub>2</sub>:CHCMe(OAc)CH<sub>2</sub>, 2,2-(methyl)lenedioxo] propyl, etc.] with PMSCl gave the corresponding isomeric productsRC<sub>2</sub>CH(SPh)CMe<sub>2</sub> and RC<sub>2</sub>CHClCMe<sub>2</sub>SPh. Hydrolysis in the presence of silica gel,

under strongly basic conditions, or dehydrochlorination under neutral or weakly basic conditions, or dehydrochlorination

under strongly basic conditions gave the hydroxy sulfides, RC<sub>2</sub>CH(SPh)CMe<sub>2</sub>OH, resp. Imethoxysulfides RC<sub>2</sub>CH(SPh)CMe<sub>2</sub> (II), or vinyl sulfides RC<sub>2</sub>C(SPh)CMe<sub>2</sub>, resp. IIwere converted to terminal trans-allylic alcs. RCH<sub>2</sub>CH:CHMe<sub>2</sub>OH.

IT 105-87-3 115-95-7 123-35-3

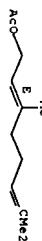
RU: RCT (Reactant); RACT (Reactant or reagent)

RN 105-87-3 HCAPLUS

(addition reaction of, with benzenesulfonyl chloride)

NAME) (CA INDEX NAME)

Double bond geometry as shown.

RN 123-35-3 HCAPLUS  
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)RN 123-35-3 HCAPLUS  
CN 1,6-Octadiene, 7-methyl-, 3-methylene- (CA INDEX NAME)H<sub>2</sub>C—CH—CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>CH<sub>2</sub>

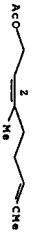
## SN 10/564307 Page 110 of 139 STIC STN SEARCH 5/17/2007

RN 141-12-8 HCAPLUS

2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)

Double bond geometry as shown.

RN 1191-16-8 HCAPLUS  
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)

RU: RCT (Reactant); RACT (Reactant or reagent)

IT 59622-99-4 66690-44-8 70473-30-2 70473-31-3

RL: RCT (Reactant); RACT (Reactant or reagent)

IT 30-10 (Terpenes and Terpenoids)

CC 105-87-3 115-95-7 123-35-3

IT 141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

141-12-8 513-35-9 1189-09-9 1191-16-8

## SN 10/564307 Page 111 of 139 STIC STN SEARCH 5/17/2007

prepared via coupling of the  $\pi$ -allylnickel halide complex derived from  $\text{Me}_2\text{C}(\text{CH}_2)\text{Br}$  with  $\text{BrCH}_2\text{CMe}(\text{CH}_2\text{CH}_2\text{C}(\text{Me})=\text{CH}_2)$  (II) or similar reaction of the  $\pi$ -allylnickel

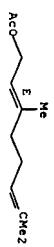
complex derived from II with QBR, resp.

IT 105-87-3 141-12-8  
RL: RCT (Reactant); RACT (Reactant or reagent)

(Grignard reaction of, with (bromomethyl)furan)

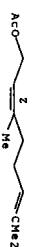
RN 105-87-3 HCAPIUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 141-12-8 HCAPIUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



IT 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of)

RN 123-35-3 HCAPIUS  
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



IT 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Glycidation of, with (bromomethyl)furan)

IT 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of)

IT 174 ANSWER 50 OF 67 HCAPIUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1983-454028 HCAPIUS Full-text  
DOCUMENT NUMBER: 99154928

TITLE: Allyl chlorides

PATENT ASSIGNEE(S): Nissui Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokyo Koho, 5 pp.

DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

## SN 10/564307 Page 112 of 139 STIC STN SEARCH 5/17/2007

JP 58052231 A 19830326 JP 1981-149226  
1981 0921

PRIORITY APPLN. INFO.: JP 1981-149226  
<-->  
1981 0921

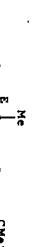
ED Entered STN: 12 May 1984  
AB RCH<sub>2</sub>HC(=CH<sub>2</sub>)CH<sub>2</sub> (R = terpenyl group) (I) were prepared by reaction of RCH<sub>2</sub>CH=CH<sub>2</sub>R1  
(R1 = H, Cl, OH, O<sub>2</sub>SCH<sub>2</sub>Ar-P, O<sub>2</sub>SPh) with trichloroisocyanuric acid. Thus, 1.0 g  
trichloroisocyanuric acid was added to 39.20 g geranyl acetate in hexane over 30 min,  
the resulting mixture kept at -5 to 0° for 1 h, and more trichloroisocyanuric acid  
added at the same temperature until no more unreacted geranyl acetate was detected by  
99s chromatog. to give 43.53 g I (R = AcOCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>).

IT 105-87-3 123-35-3 141-12-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of, by trichloroisocyanuric acid)

IT 105-87-3 HCAPIUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

IT 123-35-3 HCAPIUS  
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

Double bond geometry as shown.



IT 141-12-8 HCAPIUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



IT 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of, by trichloroisocyanuric acid)

IT 174 ANSWER 51 OF 67 HCAPIUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1983-53189 HCAPIUS Full-text

DOCUMENT NUMBER:

Carboxylic acid esters

TITLE: 90:53189

INVENTOR(S): Schlieppenhoft, Bernhard; LeBlanc, Hans;

Mallmann, Karl Heinz;

EC Erdölechemie G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 38 pp.

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

German

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3105399	A1	1981021	DE 1981-3105399	1981 0214

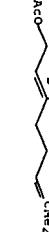
## PRIORITY APPLN. INFO.:

&lt;--&gt;

RN

CN

RN



Double bond geometry as shown.

RN

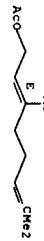
CN

SN 10/564307 Page 115 of 139 STIC STN SEARCH 5/17/2007

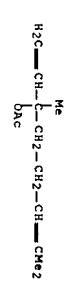
(reaction of, with sodium toluenesulfinate, catalytic)

RN 105-87-3 HCAPLUS  
2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX  
NAME)

Double bond geometry as shown.

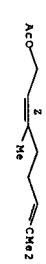


RN 115-95-7 HCAPLUS  
1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 141-12-8 HCAPLUS  
2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX  
NAME)

Double bond geometry as shown.



IT 78-79-5, reactions 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with toluenesulfinic acid, catalytic)

RN 78-79-5 HCAPLUS  
1,3-Butadiene, 2-methyl- (CA INDEX NAME)

CC 23-17 (Aliphatic Compounds)  
Section cross-references(s): 22, 25  
IT 105-87-3 115-95-7 141-12-8  
2409-88-4  
RL: RCT (Reactant); RACT (Reactant or reagent)

SN 10/564307 Page 116 of 139 STIC STN SEARCH 5/17/2007

(reaction of, with sodium toluenesulfinate, catalytic)

IT 78-79-5, reactions 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with toluenesulfinic acid, catalytic)

174 ANSWER 53 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1981:495715 HCAPLUS Full-text  
DOCUMENT NUMBER: 95:95715

TITLE: Use of 1,3,5,5-tetramethyl-2-2-oxabicyclo[2.2.2]octane in augmenting or  
enhancing the aroma or taste of foods

Sprecker, Mark A.; Schmitt, Frederick L.;  
Vock, Manfred H.; Vinals, Joaquin F.; Kiwala,  
Jacob

International Flavors and Fragrances Inc., USA  
U.S., 21 PP. Cont.-in-part of U.S. 4,195,099.  
CODEN: USXAM Patent

PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA

SOURCE: SOURCE: CODEN: USXAM  
DOCUMENT TYPE: Document  
LANGUAGE: English

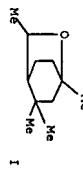
FAMILY ACC. NUM. COUNT: 5  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4269962	A	19801026	US 1979-77539	19790921
US 4195099	A	19800325	US 1978-953128	19781020
US 4203947	A	19800520	US 1979-8925	19790202
US 4283576	A	19810811	US 1979-100528	19791205
US 4267067	A	19810512	US 1980-176093	19800807
US 4289705	A	19810915	US 1980-176050	19800807
US 4303725	A	19811201	US 1980-176092	19800807
US 4320771	A	19820323	US 1980-176112	19800807

PRIORITY APPN. INFO.:  
US 1978-953128 A2  
19781020

US 1977-850845 A3  
19771111  
US 1979-8925 A3

1979  
0202  
US 1979-52334 A3 1979  
0627  
<-->  
US 1979-77539 A3 1979  
0921  
<-->



AB 1,3,5,5-tetramethyl-2-exabicyclo[2.2.2]octane (I) [78474-70-1] is prepared and used to give a fresh or nutty flavor to food, tobacco, pharmaceuticals, and other products.

Thus, mesityl oxide [141-19-7] in a suspension of AlCl<sub>3</sub> in MePh was reacted with isoprene [78-79-5] to yield 4-acetyl-1,3,3-trimethyl-1-cyclohexene-4-ethanol [55625-36-8].

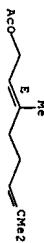
The latter was reduced with NaBH<sub>4</sub> to give 1,3,3-trimethyl-1-cyclohexene-4-ethanol [7874-71-2] which was reacted with iso-Pinol [67-63-0] and H<sub>2</sub>SO<sub>4</sub> to yield I. A

eucalyptus oil flavor formulation showed more natural eucalyptus flavor as well as a pleasant citrus nuance and sour effect when I was included at 200 ppm.

IT 105-87-3 141-12-8  
RU: BIOL (Biological study)  
(flavoring material containing tetramethyloxabicyclooctane and)

RN 105-87-3 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX  
NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX  
NAME)

Double bond geometry as shown.



IT 78-79-5 reactions  
RU: RCT (Reactant); RACT (Reactant or reagent)

AB Geranyl cyanide reacted with the bromo ketones I (R = R<sub>1</sub> = Br, Cl; R = Br<sup>2</sup>, R<sub>1</sub> = Me) to give a mixture of Me<sub>2</sub>CBrHCBr(CH<sub>2</sub>)<sub>2</sub>CMe:CHC<sub>2</sub>CN, CH<sub>2</sub>:CMeHCBr(CH<sub>2</sub>)<sub>2</sub>CMe:CHCH<sub>2</sub>CN, and

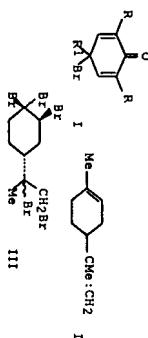
1979  
0202  
RN 78-79-5 HCAPLUS  
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)  
H<sub>3C</sub>-CH=CH-CH<sub>2</sub>

IC A231001-226  
INCL 42633600  
CC 17-2 (Foods)  
Section cross-reference(s): 62, 63  
IT Flavoring materials  
IT 75-01-6, biological studies 78-70-6 80-56-8 87-44-5  
92-22-4, biological studies 94-62-2 98-55-5 99-49-0  
99-66-5 105-87-3 110-89-4, biological studies 118-71-8 120-57-0 121-32-4 121-33-5 123-11-5, biological  
studies 127-91-3 138-95-3 141-12-8 470-02-6  
495-91-0 555-10-2 586-62-9 1329-99-3 4674-50-4 5392-40-5  
1455-54-7 38049-26-2  
RU: BIOL (Biological study)  
IT [flavoring material containing tetramethyloxabicyclooctane and]  
IT 78-79-5, Reactions  
RU: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with mesityl oxide)

L74 ANSWER 54 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1980:568119 HCAPLUS Full-text  
DOCUMENT NUMBER: 93:168419  
TITLE: Cyclization of polyenes. Part 32. Selective  
bromination of polyenes by 2,4,4,6-tetrabromocyclohexa-2,5-dieneone

AUTHOR(S): Kato, Toshihiro; Ichinose, Isao  
CORPORATE SOURCE: Dep. Chem., Tohoku Univ., Sendai, 980, Japan  
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1977-1999) (1980), (5), 1051-6  
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 93:168419  
ED Entered STN: 12 May 1984  
GI



SN 10/564307 Page 119 of 139 STIC STN SEARCH 5/17/2007

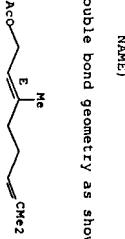
BrCH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>2</sub>)<sub>2</sub>CH=CHCH<sub>2</sub>CN with the former predominating in yields of 98, 40, and 45%, resp. This mild selective bromination was extended to a range of polyenes using CTAB and I (R = R<sub>1</sub> = Br). E.g., the polyene II gave 87% III. The di- or tetrabromo products are formed by sequential reactions.

IT

105-87-3 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)

RN

105-87-3 HCAPLUS  
2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)



Double bond geometry as shown.

RN 123-35-3 HCAPLUS  
1,6-Octadiene, 7-methyl-3-methylen- (CA INDEX NAME)



CC 30-10 (Terpenoids)  
Section cross-reference(s): 23, 24  
IT 100-42-5 reactions 105-87-3 110-83-8 reactions  
122-35-3 126-91-0 1189-09-9 4176-77-6 5989-27-5  
6495-01-1 21677-96-3 36237-88-0 42207-88-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(bromination of, by tetrabromocyclohexadienone, selective)

L74 ANSWER 55 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN

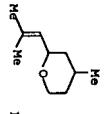
ACCESSION NUMBER: 1980:195109 HCAPLUS Full-text

DOCUMENT NUMBER:

TITLE:

The reaction of hypochlorous acid with  
olefins. A convenient synthesis of allylic  
chlorides  
Heide, Shirishar G.; Vogel, Martin K.; Saddler,  
Robert; Oliver, Michael; Woiniky, Joseph  
DEP: Chem., Purdue Univ., West Lafayette, IN,  
47907, USA  
Tetrahedron Letters (1980), 21(5),  
431-4  
CODEN: TLEAY; ISSN: 0040-4039

AUTHOR(S):  
CORPORATE SOURCE:  
SOURCE:  
DOCUMENT TYPE:  
LANGUAGE:  
ED Entered STN: 12 May 1984  
GI



SN 10/564307 Page 120 of 139 STIC STN SEARCH 5/17/2007

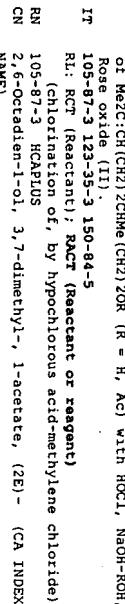
AB HOCl reacts with highly substituted olefins in CH<sub>2</sub>Cl<sub>2</sub> to give allylic chlorides. E.g., Me<sub>2</sub>C(CH<sub>2</sub>)<sub>2</sub>CH=C(R (R = CHO, CO<sub>2</sub>Me, CH<sub>2</sub>OH, CH<sub>2</sub>OAc) reacted with HOCl to give 60-80% CH<sub>2</sub>:CHMeHOCl (CH<sub>2</sub>)<sub>2</sub>CH=C(R (I)). The utility of the reaction is illustrated by preparation of a-monoterpenes and Rose oxide. Thus, sequential treatment of I (R = CHO, CO<sub>2</sub>Me, CH<sub>2</sub>OH) with Zn-TIF<sub>4</sub> and H<sub>2</sub>SO<sub>4</sub> gave CH<sub>2</sub>:CH(CH<sub>2</sub>)<sub>2</sub>OR (R = H, Ac) with HOCl, NaOH-ROH, and H<sub>2</sub>SO<sub>4</sub> gave approx. 50% Rose oxide (II).

IT

105-87-3 123-35-3 150-84-5  
RL: RCT (Reactant); RACT (Reactant or reagent)

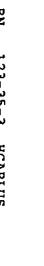
RN

105-87-3 HCAPLUS  
2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)



Double bond geometry as shown.

RN 123-35-3 HCAPLUS  
1,6-Octadiene, 7-methyl-3-methylen- (CA INDEX NAME)



CC 30-10 (Terpenoids)  
Section cross-reference(s): 23  
IT 78-70-5 89-79-2 99-99-0 105-87-3 106-22-9  
106-24-1 106-23-2 123-35-3 141-27-5 150-84-5  
591-49-1 1189-09-9 1189-92-2 4602-84-0 712-44-4  
1346-78-9 55298-92-5 5665-54-6 7451-15-1 7451-4-23-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of, by hypochlorous acid-methylene chloride)

L74 ANSWER 56 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1973:508091 HCAPLUS Full-text

DOCUMENT NUMBER:

TITLE:

A facile functionalization of the  
isopropylidene terminus of isoprenoids.  
application to the synthesis of terminal trans  
allylic alcohols  
Masaki, Yukio; Hashimoto, Kinji; Kaji, Kenji  
Gifu Coll. Pharm., Gifu, Japan



SOURCE:

*Tetrahedron Letters* (1978), (46), 4539-42

Journal

CODEN: TELEAY

ISSN: 0040-4039

DOCUMENT TYPE:

Journal

LANGUAGE:

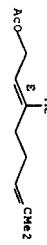
English

ED Entered STN: 12 May 1984  
 AB trans-PtichOC(=O)CH<sub>2</sub>CH=C(Me)(CH<sub>2</sub>)<sub>2</sub>CH(R<sub>1</sub>) (I; R<sub>1</sub> = CH<sub>3</sub>) on addition reaction with PhSCl, followed by dehydrochlorination in DMF (60°, 20 h) or silica gel treatment and dehydrogenation, gave I (R = SPH, R<sub>1</sub> = CH<sub>2</sub>) which on oxidation and treatment with (MeO)<sub>3</sub>P gave I' [R'R<sub>1</sub> = trans-C(CH<sub>2</sub>OH)Me] stereospecifically [76% from I (R<sub>1</sub> = CH<sub>2</sub>)]. Other terminal trans allylic acids, were prepared (47-80%) from isoprenooids by similar functionalization of the isopropylidene terminus.

IT 105-87-3 115-95-7 123-35-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (addition reaction of, with benzenealuenyl chloride)

RN 105-87-3 HCAPLUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

a-CO-CH<sub>2</sub>-CH=CH<sub>2</sub>

DOCUMENT TYPE:

Journal

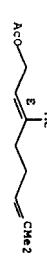
LANGUAGE:

English

CC 30-10 (Terpenoids)  
 ED Section cross-references(s): 23  
 AB 105-87-3 115-95-7 123-35-3  
 IT 141-12-8 556-82-1 1181-66-8 22089-60-7  
 5218-73-5 5324-60-7 55802-98-7 59632-99-4 68690-44-8  
 70573-30-2 70473-31-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (addition reaction of, with benzenesulfonyl chloride)

RN 174 ANSWER 57 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESION NUMBER: 1978-7078 HCAPLUS Full-text  
 DOCUMENT NUMBER: 88-7078  
 TITLE: Highly stereoselective synthesis of nerol and geraniol

AUTHOR(S): Takabe, Kunihiro; Katagiri, Takao; Tanaka, Juntao  
 SOURCE: Fac. Eng., Shizuoka Univ., Hamamatsu, Japan  
 Chemistry letters (1977), (9), 1025-6  
 CODEN: CHLTAG; ISSN: 0366-7022



DOCUMENT TYPE:

Journal

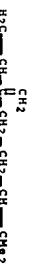
LANGUAGE:

English

ED Entered STN: 12 May 1984  
 AB Nerol was prepared stereoselectively by telomerization of isoprene in the presence of dialkylamine followed by treatment with ClCO<sub>2</sub>E, conversion of (E)-Me<sub>2</sub>C:CH<sub>2</sub>Cl to the acetate, and hydrolysis of the acetate. Geraniol was synthesized similarly via (E)-Me<sub>2</sub>C:CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Me:CH<sub>2</sub>Cl from myrcene and Pr<sub>2</sub>NH.  
 IT 105-87-3P 111-12-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (Preparation) and hydrolysis of)

RN 105-87-3 HCAPLUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS  
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 541-41-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dialkyl(dimethyloctadienyl)amine)

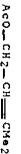


RN 141-12-8 HCAPLUS  
2,6-octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX  
NAME)

CN Double bond geometry as shown.

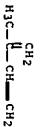


RN 1191-16-8 HCAPLUS  
2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(with amines, in presence of alkali naphthalenides)

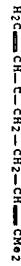
RN 78-79-5 HCAPLUS  
1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN 123-35-3 HCAPLUS  
1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 123-35-3 HCAPLUS  
1,6-Octadiene, 7-methylene- (CA INDEX NAME)



CC 23-4 (Aliphatic Compounds)  
Section cross-reference(s): 27, 28, 30

IT 105-87-3P 141-12-8P 688-92-6P  
1191-16-8P 5300-21-0P 10229-36-4P 17734-30-4P

24309-88-4P 27973-92-8P 27933-95-1P 36794-55-5P  
36794-55-5P 37857-39-9P 37857-40-2P 40137-00-6P

40267-48-9P 40267-49-0P 40267-53-6P  
51930-65-5P 51930-66-6P 51930-67-7P 51930-68-8P

51930-69-9P 51930-70-2P 51930-72-4P 51930-73-5P  
52027-04-0P 59913-90-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(Preparation of); RACT (Reactant); RACT (Reactant or reagent)

IT 78-79-5, reactions 123-35-3  
(with amines, in presence of alkali naphthalenides)

IT 174 ANSWER 62 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1974-26777 HCAPLUS Full-text  
DOCUMENT NUMBER: 80-26777  
TITLE: Unsaturated diesters

INVENTOR(S): Ono, Isao; Yanagihara, Tadaniss; Okeda, Hikaku; Koga, Toshikuni,  
Topo Soda Manuring Co., Ltd.  
SOURCE: Jpn. Tokyo Koho, 4 pp.  
COPEN: JAXXAD  
Patent  
Japanese

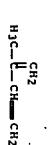
DOCUMENT TYPE:  
LANGUAGE:  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48028889	B	19730905	JP 1968-50547	1968-12-12
			JP 1968-90547	1968-12-12

ED Entered STN: 12 May 1984  
AB 2-Butene-1,4-diol esters acyclic or cyclic, with alkyl substituents or none, were obtained by reaction of conjugated dienes with carboxylic acids in the presence of Pd salt(s), transition metal salts, and alkali or alkaline metal salts. Thus, 16.3 g butadiene, 100 g AcOH, 0.65 g Pd(OAc)2, 15.0 g Cu(OAc)2, and 10.9 g NaOAc was treated at 80° under 15 atm O<sub>2</sub> for 3 hr to give 14.5 g 1,4-diacetoxyl-2-butene, 3,5-dipropionyloxy-1-cyclopentene, and 3,6-diformyloxy-1-cyclohexene.

IT 78-79-5, reactions 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(addition to, of carboxylic acids, catalysts for)

RN 78-79-5 HCAPLUS  
1,3-Butadiene, 2-methyl- (CA INDEX NAME)



IT 127-0-9-3  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts, with cupric and palladium acetates, for addition of acetic acid to butadienes)

RN 127-09-3 HCAPLUS  
Acetic acid, sodium salt (1:1) (CA INDEX NAME)

CN Acetic acid, sodium salt (1:1) (CA INDEX NAME)

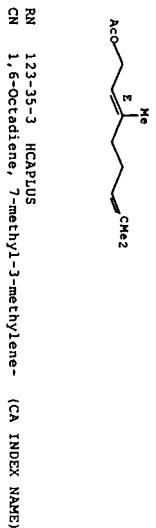
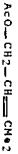


IC C07C  
CC 23-17 (Aliphatic Compounds)  
Section cross-reference(s): 24  
IT Ester, preparation  
RL: PREP (Preparation)  
(unsatd. di-)

## SN 10/564307 Page 131 of 139 STIC STN SEARCH 5/17/2007

## SN 10/564307 Page 132 of 139 STIC STN SEARCH 5/17/2007

RU: RCT (Reactant); RACT (Reactant or reagent)  
 (terpenoids from isoprene and)  
 RN 1191-16-8 HCAPLUS  
 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (terpenoids from propyl acetate and)  
 RN 78-79-5 HCAPLUS  
 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



CC 30 (Terpenoids) 105-87-3 122-33-3 2306-78-7, 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate  
 IT 80-25-2 P 16,09-44-2 P 24604-60-2 P 25905-14-0 P  
 33043-18-4 P 33443-20-8 P  
 RL: SEN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 1191-16-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (terpenoids from isoprene and)  
 IT 78-79-5, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (terpenoids from propyl acetate and)

L74 ANSWER 65 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN  
 DOCUMENT NUMBER: 1970-531138 HCAPLUS Full-text  
 73-131138  
 Complexes of terpenes with transition metals.

III. Dimerization by means of

tetrakis(triphenylphosphine)palladium

Dunne, K.; McDowell, Francis J.  
 Dep. Org. Chem., Univ. Newcastle-upon-Tyne,  
 Newcastle-upon-Tyne, UK  
 Journal of the Chemical Society [Section] C:  
 Organic (1970), (16), 2203-6  
 CODEN: JOCOMX; ISSN: 0022-4952

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

ED Entered STN: 12 May 1984

AB The esters of linanol, geranil, and nerol were prepared from myrcene. Thus, a mixture of 50 lb 80% myrcene, 200 lb AcOH, and 0.5 lb tert-butylcetohol was stirred in an inert atmospheric at 110-20° 36 hr to give 10 lb acetate esters, containing 55% geranyl and neril acetates, 15% myrcenyl acetates, and 12%  $\alpha$ -terpinyl acetate.

IT 80-26-2 P 105-87-3 P 141-12-8 P

RL: SEN (Synthetic preparation); PREP (Preparation)

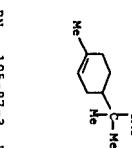
(preparation of)

RN 80-26-2 HCAPLUS

2,6-Octadien-1-ol, 3,7-dimethyl-, (2E)- (CA INDEX NAME)

NAME)

Double bond geometry as shown.

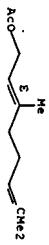




SN 10/564307 Page 133 of 139 STIC STN SEARCH 5/17/2007

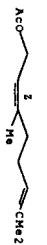
CN 2,6-octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
RN (Reaction of, with acetic acid)

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



H<sub>2</sub>C—CH—[CH<sup>CH<sub>2</sub></sup>]—CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>

IT 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
RN (Preparation of)

CN 123-35-3

IT 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with acetic acid)

L74 ANSWER 67 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1957-76161 HCAPLUS Full-text

DOCUMENT NUMBER: 66:76161  
TITLE: Dehydrogenation of monoterpenic compounds on platinum-alumina catalyst

AUTHOR(S): Mizrahi, Isaac; Nigam, Ishwar C.  
CORPORATE SOURCE: Food Drug Directorate, Ottawa, Can.  
SOURCE: Journal of Chromatography (1966), 25(2), 230-41

DOCUMENT TYPE: CODE: JOCRAM; ISSN: 0021-9673  
LANGUAGE: English  
ED Entered STN: 12 May 1984  
cf. CA 66, 75418P. Dehydrogenation of 42 monoterpenes was investigated using a reactor packed with 5% Pt on Al2O3. Products obtained were analyzed by gas chromatography on 3 instruments using a thermal conductivity detector, and a H flame ionization detector.

SN 10/564307 Page 134 of 139 STIC STN SEARCH 5/17/2007

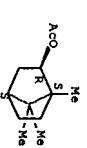
Exptl. data correlated with the structures of the parent compds. Mechanisms of dehydrogenations and isomerizations involved were discussed.

IT 76-49-3 105-87-3 115-99-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrogenation of, chromatog. and)

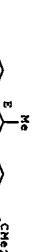
RN 76-49-3 HCAPLUS  
CN Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, 2-acetate, (1R,2S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 105-87-3 HCAPLUS  
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

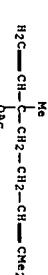
Double bond geometry as shown.



IT 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
RN (Reaction of, with acetic acid)

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



H<sub>2</sub>C—CH—[CH<sup>CH<sub>2</sub></sup>]—CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>

IT 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
RN (Preparation of)

CN 123-35-3

IT 123-35-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrogenation of, chromatog. and)

CC 30 [Terpenes] 70-76 79-92-5 80-95-8, reactions 89-98-5  
IT 76-49-3 78-76-6 99-82-1 99-83-2 99-86-5 100-86-2 105-87-3  
98-55-5 105-24-1 115-95-7 115-99-1 123-35-3  
106-22-9 106-24-1 115-95-7 115-99-1 123-35-3  
127-91-3 138-86-3 491-05-4 498-15-7 500-00-5 501-70-0  
586-62-9 586-67-4 1134-98-8 1197-07-5 1490-04-6  
1639-73-1 3387-11-5 7786-67-6 1387-91-3 2956-98-2

RN (dehydrogenation of, chromatog. and)

SEARCH HISTORY

\*\*> d his profile

(FILE 'HOME' ENTERED AT 10:23:49 ON 16 MAY 2007)

FILE 'HCAPLUS' ENTERED AT 10:24:09 ON 16 MAY 2007

L1  
1 SEA ABB=ON PLU=ON US20070055076/PN  
D ALL  
SEL RN

L2 FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007  
35 SEA ABB=ON PLU=ON (100-66-3/B1 OR 105-87-3/B1 OR  
105-90-8/B1 OR 105-91/B1 OR 106-25-2/B  
I OR 106-42-3/B1 OR 107-92-6/B1 OR 108-21-4/B1 OR  
108-88-3/B1 OR 109-90-7/B1 OR 109-92-6/B  
I OR 1191-16-8/B1 OR 123-35-3/B1 OR 123-86-4/B1 OR  
127-08-2/B1 OR 127-03-3/B1 OR 137-10-6/B1 OR 138-86-3/B  
I OR 1411-12-8/B1 OR 142-96-1/B1 OR 157258-67-8/B1 OR  
1955-9-59-/B1 OR 3915-83-1/B1 OR 503-74-2/B1 OR  
5392-45-2/B1 OR 56-49-7-/B1 OR 64-19-2/B1 OR  
78-93-3/B1 OR 79-09-4/B1 OR 79-31-2/B1 OR 80-26-2/B  
I OR 831785-97-2/B1)

L3 19 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS

L4 1 SEA ABB=ON PLU=ON 123-35-3/RN

D SCAN

D CN

D IDE

1 SEA ABB=ON PLU=ON 78-79-5/RN

D SCAN

D IDE

1 SEA ABB=ON PLU=ON 1191-16-8/RN

D SCAN

D CN

D IDE

1 SEA ABB=ON PLU=ON 105-87-3/RN

D SCAN

D IDE

1 SEA ABB=ON PLU=ON 141-12-8/RN

D IDE

L9 11 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS  
FILE 'STNGUIDE' ENTERED AT 10:44:21 ON 16 MAY 2007

L10 FILE 'CASREACT' ENTERED AT 10:54:09 ON 16 MAY 2007  
1 SEA ABB=ON PLU=ON 123-35-3/RCT(L) (105-87-3/PRO OR  
141-12-8-/RO)  
D SCAN

L11 2 SEA ABB=ON PLU=ON 78-79-5/RCT(L)1191-16-8/PRO  
D SCAN

E ESTER/CT

E ESTERS/CT

L12 23 SEA ABB=ON PLU=ON 64-19-7/RCT(L) (123-35-3/RCT OR  
78-79-5/RCT)  
D SCAN

STR 122-35-3

L13 36 SEA SSS SAM L13 ( 448 REACTIONS)

L14 709 SEA SSS FUL L13 ( 11229 REACTIONS)

SAV LIS LAQ307CRCT/A

E ESTERS/CT

L15 7147 SEA ABB=ON PLU=ON ESTERS-PFT, OLD, NT/CT  
7 SEA ABB=ON PLU=ON LIS AND L16  
D SCAN

D QUE  
D SCAN  
D QUE

SN 10/564307 Page 137 of 139 STIC STN SEARCH 5/17/2007

L18  
L19  
6 SEA SUB-L15 SSS SAM L18 ( 28 REACTIONS)  
STR L13  
D SCAN  
SAV L20 LAO307CRTC/A  
88 SEA SUB-L15 SSS FUL L18 ( 708 REACTIONS)  
STR L18  
1 SEA SUB-L15 SSS SAM L21 ( 7 REACTIONS)  
D SCAN  
D SCAN  
5 SEA SUB-L15 SSS FUL L21 ( 16 REACTIONS)  
D SCAN  
D SCAN  
SAV L23 LAO307CRTC/A  
STR L21  
1 SEA SUB-L15 SSS SAM L24 ( 7 REACTIONS)  
D SCAN  
D SCAN  
7 SEA SUB-L15 SSS FUL L24 ( 36 REACTIONS)  
D SCAN  
SAV L26 LAO307CRTC/A  
SAV L26 LAO307CRTC/A  
34 SEA ABB=ON PLU=ON (L10 OR L11 OR L12) OR L17 OR L23  
OR L26  
L28  
43 SEA ABB=ON PLU=ON BABLER JAMES?AU  
3 SEA ABB=ON PLU=ON L27 AND L28  
SAV L29 LAO307CRTC/A  
31 SEA ABB=ON PLU=ON L27 NOT L29  
FILE 'HCAPIUS' ENTERED AT 12:06:06 ON 16 MAY 2007  
QUE ABB=ON PLU=ON PY<2004 OR PRK<2004 OR AY<2004 OR  
MT<2004 OR REVENDT  
1 SEA ABB=ON PLU=ON L1 AND 131  
D SCAN  
132  
FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007  
133  
25 SEA ABB=ON PLU=ON L30 AND 131  
3 SEA ABB=ON PLU=ON L29 AND 131  
134  
FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007  
D SCAN L1  
619 SEA ABB=ON PLU=ON L4/RACT  
5537 SEA ABB=ON PLU=ON L5/RACT  
86 SEA ABB=ON PLU=ON L6/P  
137 SEA ABB=ON PLU=ON L7/P  
138 SEA ABB=ON PLU=ON L7/P  
347 SEA ABB=ON PLU=ON L7/P  
D 1-2 KWIC  
144 SEA ABB=ON PLU=ON L8/P  
D KWIC  
D 1-2 L16 KWIC  
140  
0 SEA ABB=ON PLU=ON L36(L) L37  
141  
1 SEA ABB=ON PLU=ON L36 AND L37  
142  
0 SEA ABB=ON PLU=ON L35 (L) (L38 OR L39)  
143  
1 SEA ABB=ON PLU=ON L35 AND (L38 OR L39)  
144  
20 SEA ABB=ON PLU=ON L35 (L) (L40 OR L41 OR L42 OR L43)  
145  
146  
147  
34845 SEA ABB=ON PLU=ON L35 OR (L35 OR L36) AND L45  
4036 SEA ABB=ON PLU=ON L39/RACT  
50 SEA ABB=ON PLU=ON (L35 OR L36) AND L47  
148  
9 SEA ABB=ON PLU=ON L48 AND L44  
149  
E ESTERS/CT  
E ESTERS/CT  
QUE ABB=ON PLU=ON ESTERS+PFT,OLD,NTL/CT  
70 SEA ABB=ON PLU=ON L44 OR L46 OR (L48 OR L49)  
47 SEA ABB=ON PLU=ON L51 AND L50  
E VITAMINS/CT  
QUE ABB=ON PLU=ON VITAMINS+PFT,OLD,NT/CT  
E FLAVORECT  
E FLAVORECT  
E FLAVORECT  
E FLAVORECT  
QUE ABB=ON PLU=ON FLAVOR+PFT,OLD,NT/CT

SN 10/564307 Page 138 of 139 STIC STN SEARCH 5/17/2007

L55  
3 SEA ABB=ON PLU=ON L51 AND (L53 OR L54)  
D SCAN  
D SCAN L1  
E "DIETARY SUPPLEMENTS"/CT  
QUE ABB=ON PLU=ON "DIETARY SUPPLEMENTS"+PFT,OLD,NT/CT  
QUE ABB=ON PLU=ON "FLAVORING MATERIALS"+PFT,OLD,NT/CT  
QUE ABB=ON PLU=ON "ODOR AND ODOROUS SUBSTANCES"+PFT,OLD,NT/CT  
LD,NT/CT  
45 SEA ABB=ON PLU=ON L52 AND L31  
SAV L59 LAO307HCPCA  
43 SEA ABB=ON PLU=ON L28  
D QUE  
43 SEA ABB=ON PLU=ON L60 AND L31  
L61  
L62  
QUE ABB=ON PLU=ON VITAMIN? OR ODOR? OR SMELL? OR  
PERFUME? OR SUPPLEMENT? OR FLAVOR?  
L63  
L64  
4 SEA ABB=ON PLU=ON L61 AND L62  
4 SEA ABB=ON PLU=ON L61 AND (L53 OR L56 OR L57 OR L58)  
D QUE  
L65  
5 SEA ABB=ON PLU=ON L51 AND (L53 OR L56 OR L57 OR L58)  
L66  
L67  
45 SEA ABB=ON PLU=ON L55 OR L59 OR L65  
SAV L67 LAO307HCPCA  
6 SEA ABB=ON PLU=ON L63 OR L64  
13 SEA ABB=ON PLU=ON L61 AND L50  
L70  
17 SEA ABB=ON PLU=ON L66 OR L69  
SAV L70 LAO307HCPCA  
D QUE L67  
43 SEA ABB=ON PLU=ON L67 NOT L70  
D QUE L34  
D QUE L33  
FILE 'CASREACT' ENTERED AT 12:45:36 ON 16 MAY 2007  
D QUE L33  
FILE 'STNGUIDE' ENTERED AT 12:46:03 ON 16 MAY 2007  
FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16  
MAY 2007  
L72  
4 SEA ABB=ON PLU=ON L28  
D 1-4 TT  
SAV L72 LAO307IN/A  
FILE 'STNGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007  
D QUE L34  
D QUE L70  
D QUE L72  
FILE 'CASREACT, HCAPIUS, BIOSIS' ENTERED AT 12:49:46 ON 16 MAY  
2007  
19 DUP REM L34 L70 L72 (5 DUPLICATES REMOVED)  
ANSWERS '1-3' FROM FILE CASREACT  
ANSWERS '4-18' FROM FILE HCAPIUS  
ANSWER '19' FROM FILE BIOSIS  
FILE 'CASREACT' ENTERED AT 12:51:20 ON 16 MAY 2007  
FILE 'CASREACT, HCAPIUS, BIOSIS' ENTERED AT 12:57:01 ON 16 MAY  
2007  
D L73 1-19 IBIB ABS  
FILE 'CASREACT' ENTERED AT 12:57:02 ON 16 MAY 2007  
QUE ABB=ON PLU=ON FLAVOR+PFT,OLD,NT/CT

SN 10/564307 Page 139 of 139 STIC STN SEARCH 5/17/2007

FILE 'REGISTRY' ENTERED AT 12:57:42 ON 16 MAY 2007

D 14 IDE  
D 15 IDE  
D 16 IDE  
D 17 IDE  
D 18 IDE

FILE 'STNGUIDE' ENTERED AT 12:59:34 ON 16 MAY 2007

D QUE STAT L33  
D QUE STAT L71

FILE 'CASREACT\_HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007

L74 67 DUP REM L33 L71 (1 DUPLICATE REMOVED)  
ANSWERS 1-25, FROM FILE CASREACT  
ANSWERS 26-67, FROM FILE HCAPLUS  
D 174 1-5 1B1B ABS FHT  
D 174 26-67 1B1B ED ABS HITSTR HITIND